Attachment: No

Case/Application number: 10/518,872 PALM <http://expoweb1:8001/cgi-bin/expo/GenInfo/snquery.pl?APPL_ID=10/518,872>
Priority App. Filing Date: 7/2/2002
Format for Search Results: SCORE & EMAIL

Identify the novelty:

Additional Comments:
Please search structure claim 1, amendment filed 10/1/2009. Please search ligand with any metal ion (i.e. do not limit to only Tc or Re). Thanks!

=> fil hcaplu
FILE 'HCAPLUS' ENTERED AT 15:00:12 ON 13 OCT 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 13 Oct 2009 VOL 151 ISS 16
FILE LAST UPDATED: 12 Oct 2009 (20091012/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

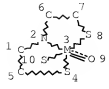
HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

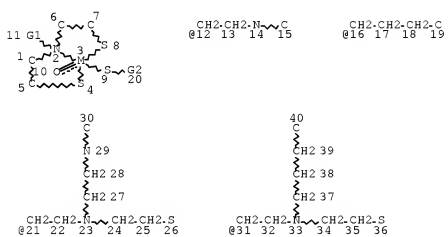
=> d stat que l8
L1 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L3 906 SEA FILE=REGISTRY SSS FUL L1
L6 STR



VAR G1=12/16
VAR G2=21/31
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE
L7 4 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L8 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

=> d ibib abs hitstr 18 1-5

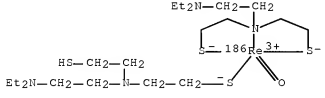
L8 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:945145 HCAPLUS Full-text

DOCUMENT NUMBER: 149:432345
TITLE: Imaging of 186Re-liposome therapy in ovarian cancer xenograft model of peritoneal carcinomatosis
AUTHOR(S): Zavaleta, Cristina L.; Goins, Beth A.; Bao, Ande; McManus, Linda M.; McMahan, C. Alex; Phillips, William T.
CORPORATE SOURCE: Department of Radiology, University of Texas Health Science Center at San Antonio, San Antonio, TX, USA
SOURCE: Journal of Drug Targeting (2008), 16(7-8), 626-637 CODEN: JDTAEH; ISSN: 1061-186X
PUBLISHER: Informa Healthcare
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This study determined the biodistribution of rhenium-186 (186Re) encapsulated in biotin-liposomes containing patent blue dye, injected i.p. with avidin in an OVCAR-3 ovarian cancer xenograft model and evaluated tumor response of this therapy with fluorine-18-fluorodeoxyglucose (18F-FDG) microPET imaging. Treated rats (n = 8) received an IP injection of 186Re-blue-biotin-liposomes (1000 MBq/kg) 30 min before an IP injection of avidin (5 mg), whereas control rats (n = 4) received a sham IP injection of saline. Scintigraphic images showed that 186Re-blue-biotin liposomes/avidin were retained in the peritoneal cavity with 18% of the original activity remaining after 5 days. From 1 to 4 wk post-treatment, peritoneal 18F-FDG standard uptake values decreased 30% in treatment group, yet increased 44% in control group. Total number of cells in ascites was significantly higher in control vs. treatment group. Omental fat in control rats had numerous tumor cells compared with treated rats. Results show the potential for 186Re-blue-biotin-liposome/avidin system in treating advanced ovarian cancer involving peritoneal carcinomatosis.

IT 644961-22-8
RL: BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(imaging of 186Re-liposome therapy in ovarian cancer xenograft model of peritoneal carcinomatosis)

RN 644961-22-8 HCAPLUS
CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:130959 HCAPLUS Full-text
DOCUMENT NUMBER: 140:327019

TITLE: Direct 99mTc labeling of pegylated liposomal doxorubicin (doxil) for pharmacokinetic and non-invasive imaging studies

AUTHOR(S): Bao, Ande; Goins, Beth; Klipper, Robert; Negrete, George; Phillips, William T.

CORPORATE SOURCE: Department of Radiology, University of Texas Health Science Center at San Antonio, San Antonio, TX, USA

SOURCE: Journal of Pharmacology and Experimental Therapeutics (2004), 308(2), 419-425
CODEN: JPETAB; ISSN: 0022-3565

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

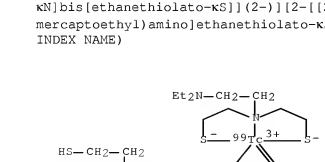
LANGUAGE: English

AB Pharmacokinetic and organ distribution studies of liposomal drugs in humans are a challenge. A direct labeling method using 99mTc-N,N-bis(2-mercaptoethyl)-N',N'-diethyl-ethylenediamine (BMEDA) complex to label the com. available pegylated liposomal doxorubicin, Doxil, has been introduced. Biodistributions of 99mTc-Doxil in normal rats were performed to evaluate the feasibility of using it for monitoring the pharmacokinetics of liposomes encapsulating drugs. Labeling efficiency of 99mTc-Doxil was 70.6 ± 0.8% (n = 3). In vitro incubation of 99mTc-Doxil in 50% fetal bovine serum or 50% human serum at 37℃ showed good labeling stability with 72.3 ± 3.6% or 78.6 ± 1.8% of activity associated with Doxil at 24 h, resp. (n = 3). There was a two-phase blood clearance with half-clearance times of 2.2 and 26.2 h after bolus i.v. injection in normal rats. Distribution of 99mTc-Doxil at 44 h after injection had 19.8 ± 1.3% of injected dose in blood, 14.1 ± 1.7% in liver, 2.6 ± 0.3% in spleen, 9.0 ± 0.8% in bone with marrow, 6.0 ± 0.5% in skin, and 15.3 ± 4.3% in bowel (n = 5). Unencapsulated 99mTc-BMEDA had a very rapid blood clearance with a half-clearance time of only 0.12 h (n = 4). By using this 99mTc labeling method, biodistribution and pharmacokinetics of ammonium gradient liposomes encapsulating drugs can be determined by noninvasive scintigraphic imaging. This labeling method may be extended to 186Re and 188Re labeling to combine chemotherapy and radionuclide therapy for tumor treatment.

IT 644961-20-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(direct 99mTc labeling of pegylated liposomal doxorubicin (doxil) for pharmacokinetic and non-invasive imaging studies)

RN 644961-20-6 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS

RECORD (22 CITINGS)
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:41205 HCAPLUS Full-text
DOCUMENT NUMBER: 140:99594
TITLE: Radiolabeled compounds and liposomes and their methods of making and using the same
INVENTOR(S): Bao, Ande; Phillips, William T.; Goins, Beth
PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004004635	A2	20040115	WO 2003-US16363	20030522
WO 2004004635	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2490959	A1	20040115	CA 2003-2490959	20030522
AU 2003241598	A1	20040123	AU 2003-241598	20030522
EP 1536843	A2	20050608	EP 2003-731347	20030522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 20050222396	A1	20051006	US 2005-518872	20050617

PRIORITY APPLN. INFO.: US 2002-393619P P 20020702
WO 2003-US16363 W 20030522

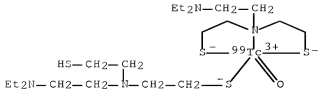
OTHER SOURCE(S): MARPAT 140:99594

AB The invention relates to radiolabeled compds. and, in particular, complexes of 99mTc or 186Re incorporated into liposomes along with thiol compds. and other drugs (such as doxorubicin). The invention also relates to kits for preparing the radiolabeled liposomes which are useful for imaging and radiotherapy.

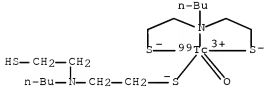
IT 644961-20-6P 644961-21-7P 644961-22-8P
644961-23-9P
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(radiolabeled liposomes containing thiols and other drugs as imaging and radiotherapeutic agents)

RN 644961-20-6 HCAPLUS

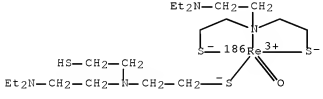
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



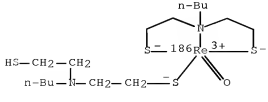
RN 644961-21-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-[butyl(2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 644961-22-8 HCAPLUS
CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 644961-23-9 HCAPLUS
CN Rhenium-186Re, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-[butyl(2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

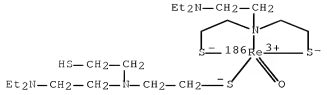
L8 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:32039 HCAPLUS Full-text
DOCUMENT NUMBER: 141:265682
TITLE: 186Re-liposome labeling using 186Re-SNS/S complexes: in vitro stability, imaging, and biodistribution in rats
AUTHOR(S): Bao, Ande; Goins, Beth; Klipper, Robert; Negrete, George; Phillips, William T.
CORPORATE SOURCE: Department of Radiology, University of Texas Health Science Center at San Antonio, San Antonio, TX, USA
SOURCE: Journal of Nuclear Medicine (2003), 44(12), 1992-1999
CODEN: JNMEAQ; ISSN: 0161-5505
PUBLISHER: Society of Nuclear Medicine
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Liposomes are important carriers for controlling the spatial and temporal distribution of drug mols. or other bioactive mols. Radiolabeled liposomes have potential applications in diagnostic imaging and radionuclide therapy. The purpose of this study was to develop a practical method for labeling liposomes with therapeutic rhenium radionuclides, using 186Re as an example. Methods: An SNS pattern ligand, N,N-bis(2-mercaptoethyl)-N',N'-diethylethylenediamine (BMEDA), and an S pattern ligand, benzene thiol (BT), were used to make 2 kinds of 186Re-SNS/S complexes, 186Re-BMEDA and 186Re-BMEDA + BT. These 186Re-SNS/S complexes were mixed with neutral liposomes encapsulating cysteine or (NH4)2SO4 to prepare 186Re-liposomes. The in vitro labeling stability of 186Re-liposomes was investigated by incubation in 50% fetal bovine serum/50% phosphate-buffered saline, pH 7.4, at 37°C. Rat distribution studies of 186Re-liposomes after i.v. injection were also performed. Results: The labeling efficiencies of 186Re-liposomes were 52.9%-81.3% depending on the 186Re-SNS/S complex chosen and whether cysteine- or (NH4)2SO4-encapsulated liposomes were used. 186Re-(NH4)2SO4 liposomes labeled with 186Re-BMEDA had the best in vitro labeling stability in serum with 89.8% ± 3.1% of the radioactivity associated with liposomes at 24 h and 76.2% ± 5.1% at 96 h. A specific activity of 1.85 GBq (50 mCi) of 186Re per 50 mg of phospholipid could be achieved with good labeling stability. Biodistributions were followed for 72 h and showed good in vivo stability for 186Re-liposomes that was characterized by a slow blood clearance and a gradually increasing spleen accumulation. 186Re-BMEDA alone had fast blood clearance and no accumulation in spleen. Conclusion: A practical method for labeling liposomes with 186Re using 186Re-SNS/S complexes is described. The labeled 186Re-liposomes were stable in serum and in vivo and could potentially be useful for radionuclide therapy.

IT 644961-22-8P
RL: DGN (Diagnostic use); PEP (Physical, engineering or chemical process); PKT (Pharmacokinetics); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(186Re-liposome labeling using 186Re-SNS/S complexes)

RN 644961-22-8 HCAPLUS

CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:718547 HCAPLUS Full-text
DOCUMENT NUMBER: 140:292608
TITLE: A novel liposome radiolabeling method using 99mTc-"SNS/S" complexes: In vitro and in vivo evaluation
AUTHOR(S): Bao, Ande; Goins, Beth; Klipper, Robert; Negrete, George; Mahindaratne, Mathew; Phillips, William T.
CORPORATE SOURCE: Department of Radiology, University of Texas Health Science Center at San Antonio, San Antonio, TX, 78229-3900, USA
SOURCE: Journal of Pharmaceutical Sciences (2003), 92(9), 1893-1904
CODEN: JPMSAE; ISSN: 0022-3549
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

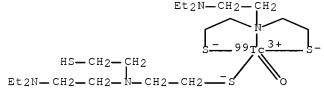
AB Liposomes are important carriers for controlled drug release, for gene or antisense therapy, and for immunization. Radiolabeled liposomes can be used to evaluate the in vivo behavior of different liposome formulations, as well as for diagnostic imaging and radionuclide therapy. A novel method for radiolabeling liposomes with 99mTc-"SNS/S" complexes is introduced. This labeling method can be applied to liposome radiolabeling with not only 99mTc but also two therapeutic radionuclides, 186Re and 188Re. Liposomes encapsulating glutathione (GSH) were studied for 99mTc labeling. N,N-bis(2-mercaptoethyl)-N',N'-diethyl-ethylenediamine (BMEDA), N,N-bis(2-mercaptoethyl)-1-butylamine (BMBuA), and benzene thiol (BT) were investigated to make 99mTc-"BMEDA", 99mTc-"BMEDA + BT", 99mTc-"BMBuA", and 99mTc-"BMBuA + BT", for liposome labeling. The labeling efficiencies of 99mTc-GSH liposomes were from 36.9 to 69.2%. After incubation in serum, 99mTc-GSH liposomes labeled with 99mTc-"BMEDA" or 99mTc-"BMEDA + BT" had the best labeling stability of the formulations tested. Distribution studies after i.v. injection of 99mTc-liposomes composed of distearoyl phosphatidylcholine (DSPC) and cholesterol had a slow blood clearance and a high spleen accumulation demonstrating the in vivo labeling stability of the radiolabeled liposomes. The 99mTc-liposomes have great potential as a radiopharmaceutical system for evaluating various kinds of liposomes with different lipid composition, for evaluating in advance a subsequent radionuclide therapy using 186Re or 188Re labeled liposomes and for diagnostic imaging.

IT 644961-20-6P 644961-21-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, stability and biodistribution of liposomes radiolabeled with 99mTc-mixed ligand complexes)

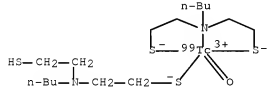
RN 644961-20-6 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][2-[[2-(diethylamino)ethyl](2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 644961-21-7 HCAPLUS

CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-[butyl(2-mercaptoethyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

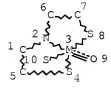


OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => d stat que l13

L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

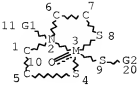
DEFAULT ECLEVEL IS LIMITED

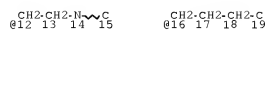
GRAPH ATTRIBUTES:

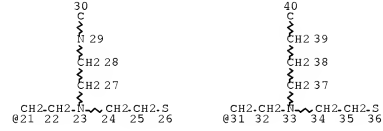
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L3 906 SEA FILE=REGISTRY SSS FUL L1
L6 STR



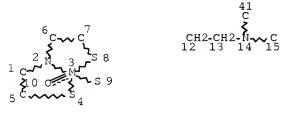




VAR G1=12/16
VAR G2=21/31
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE
L7 4 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L9 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L10 177 SEA FILE=REGISTRY SUB=L3 SSS FUL L9
L11 173 SEA FILE=REGISTRY ABB=ON PLU=ON L10 NOT L7

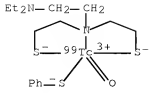
```
L12          61 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L13          52 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L12 AND (AY=<2002 OR PY=<2002
                OR PRY=<2002 OR PD=< AUGUST 2, 2002)


=> d ibib abs hitstr l13 1-52

L13  ANSWER 1 OF 52  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2004:41205  HCAPLUS  Full-text
DOCUMENT NUMBER:          140:99594
TITLE:                    Radiolabeled compounds and liposomes and their methods
                          of making and using the same
INVENTOR(S):              Bao, Ande; Phillips, William T.; Goins, Beth
PATENT ASSIGNEE(S):       Board of Regents, the University of Texas System, USA
SOURCE:                   PCT Int. Appl., 75 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
     --------------        ----   --------    -------------------      --------
     WO 2004004635          A2    20040115    WO 2003-US16363          20030522 <--
     WO 2004004635          A3    20040701
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2490959             A1    20040115    CA 2003-2490959          20030522 <--
     AU 2003241598          A1    20040123    AU 2003-241598           20030522 <--
     EP 1536843             A2    20050608    EP 2003-731347           20030522 <--
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     US 20050222396         A1    20051006    US 2005-518872           20050617 <--
PRIORITY APPLN. INFO.:                         US 2002-393619P      P   20020702 <--
                                               WO 2003-US16363      W   20030522

OTHER SOURCE(S):          MARPAT 140:99594
AB   The invention relates to radiolabeled compds. and, in particular, complexes of
     99mTc or 186Re incorporated into liposomes along with thiol compds. and other
     drugs (such as doxorubicin).  The invention also relates to kits for preparing
     the radiolabeled liposomes which are useful for imaging and radiotherapy.
IT   644961-29-5P
     RL: DGN (Diagnostic use); PKT (Pharmacokinetics); PRP (Properties); SPN
     (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (radiolabeled liposomes containing thiols and other drugs as imaging and
        radiotherapeutic agents)
RN   644961-29-5  HCAPLUS
CN   Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-
     κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI)  (CA
     INDEX NAME)
```



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:89450 HCAPLUS Full-text
DOCUMENT NUMBER: 137:275074
TITLE: Novel mixed ligand technetium complexes as 5-HT1A receptor imaging agents
AUTHOR(S): Leon, A.; Rey, A.; Mallo, L.; Pirmettis, I.; Papadopoulos, M.; Leon, E.; Pagano, M.; Manta, E.; Incerti, M.; Raptopoulou, C.; Terzis, A.; Chiotellis, E.
CORPORATE SOURCE: Catedras de Radioquimica y Quimica Farmaceutica, Facultad de Quimica, Montevideo, Urug.
SOURCE: Nuclear Medicine and Biology (2002), 29(2), 217-226
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis, characterization and biol. evaluation of two novel 3 +1 mixed ligand 99mTc-complexes, bearing the 1-(2-methoxyphenylpiperazine) moiety, a fragment of the true 5-HT1A antagonist WAY 100635, is reported. Complexes at tracer level 99mTcO[(CH3CH2)2NCH2CH2N(CH2CH2S)2][o-CH3OC6H4N(CH2CH2)2NCH2CH2S], 99mTc-1, and 99mTcO[((CH3)2CH)2NCH2CH2N(CH2CH2S)2][o-CH3OC6H4N (CH2CH2)2NCH2CH2S], 99mTc-2, were prepared using 99mTc-glucoheptonate as precursor. For structural characterization, the analogous oxorhenium complexes, Re-1 and Re-2, were prepared by ligand exchange reaction using ReOCl3(PPh3)2 as precursor, and characterized by elemental anal. and spectroscopic methods. Complex Re-1 was further characterized by crystallog. anal. Labeling was performed with high yield (>85%) and radiochem. purity (>90%) using very low ligand concentration The structure of 99mTc complexes was established by comparative HPLC using the well-characterized oxorhenium analogs as refs. In vitro binding assays demonstrated the affinity of these complexes for 5-HT1A receptors (IC50 : 67 and 45 nM for Re-1 and Re-2 resp.). Biol. studies in mice showed the ability of 99mTc-1 and 99mTc-2 complexes to cross the intact blood-brain barrier (1.4 and 0.9% dose/g, resp. at 1 min post-inj.). The distribution of these complexes in various regions in rat brain is inhomogeneous. The highest ratio between areas reach and poor in 5-HT1A receptors was calculated for complex Tc-1 at 60 min p.i. (hippocampus/cerebellum = 1.7).

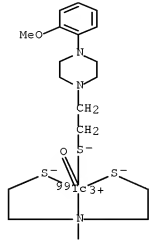
IT 449142-18-1P 464878-67-9P
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(mixed ligand 99mTc-complexes preparation and evaluation as 5-HT1A receptor

imaging agents)

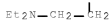
RN 449142-18-1 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(2-methoxyphenyl)-1-piperazineethanethiolato-κS1]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A



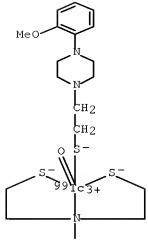
PAGE 2-A



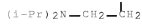
RN 464878-67-9 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(2-methoxyphenyl)-1-piperazineethanethiolato-κS1]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A

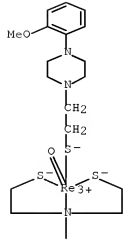


PAGE 2-A

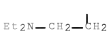


IT 464878-68-0P 464878-69-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mixed ligand 99mTc-complexes preparation and evaluation as 5-HT1A receptor imaging agents)
RN 464878-68-0 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(2-methoxyphenyl)-1-piperazineethanethiolato-κS1]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A

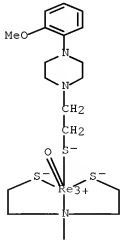


PAGE 2-A



RN 464878-69-1 HCAPLUS
CN Rhenium, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(2-methoxyphenyl)-1-piperazineethanethiolato-κS1]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

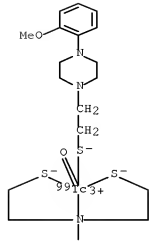
L13 ANSWER 3 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:931938 HCAPLUS Full-text
DOCUMENT NUMBER: 137:190664
TITLE: Synthesis and biodistribution of 5-HT1A receptor imaging agent with 99Tcm
AUTHOR(S): Liu, Fei; He, Youfeng; Luo, Zhifu; Liu, Yingmei
CORPORATE SOURCE: Department of Isotope, China Institute of Atomic Energy, Beijing, 102413, Peop. Rep. China
SOURCE: Tongweisu (2001), 14(3-4), 129-135
CODEN: TONGEM; ISSN: 1000-7512
PUBLISHER: Yuanzineng Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB 99Tcm complexes for 5-HT1A receptor imaging agents were prepared The compds. 1-(2-methoxyphenyl)-4-(2- mercaptoethyl)piperazine (MPMEP) as a monodentate, N,N-bis(2- mercaptoethyl)-N',N'-diethylethylenediamine (BMPDEEDA) and N,N-bis(2-mercaptoethyl)benzylamine (BMPBA) as tridentate were synthesized and characterized by IR, 1HNMR. Two compds. 99TcmO (MPMEP) (BMPDEEDA) and 99TcmO (MPMEP) (BMPBA) complexes were prepared via "3+1" mixed-ligand approach by using 99Tcm-glucoheptonate as precursor. Monodentate and tridentate concentration, reaction time, pH, and temperature of the reaction system were optimized to achieve high labeling yield: pH 6.0-7.0, reaction temperature 60-70° and reaction time 20-30 min, the labeling yield of the 99TcmO (BMPDEEDA) and 99TcmO (MPMEP) (BMBA) was 95% and 90% after extraction by CH2Cl2. The reaction mixture was analyzed and separated by HPLC system, and radiochem. purity was more than 98%. Biodistribution of two 99Tcm mixed-ligand complexes in mice demonstrated that they can penetrate the blood brain barrier and have a high brain uptake and retention for a certain time in brain. The ratio of brain and blood uptake was 0.32 and 0.198 after administration 60 min for 99TcmO (MPMEP) (BMPBA) and 99TcmO (MPMEP) (BMPDEEDA), resp. The radioactivity clearance form blood of 99TcmO (BMPBA) was rapid, but radioactivity level in blood was even high.

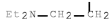
IT 449142-18-1P
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and biodistribution of 5-HT1A receptor imaging agent with 99Tcm)

RN 449142-18-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(2-methoxyphenyl)-1-piperazineethanethiolato-κS1]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L13 ANSWER 4 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:407940 HCAPLUS Full-text
DOCUMENT NUMBER: 135:28327
TITLE: Dopamine and serotonin transporter ligands and imaging agents
INVENTOR(S): Kung, Hank; Meegalla, Sanath; Kung, Mei-ping; Plossl, Karl
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA
SOURCE: U.S., 53 pp., Cont.-in-part of U.S. Ser. No. 545,327, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

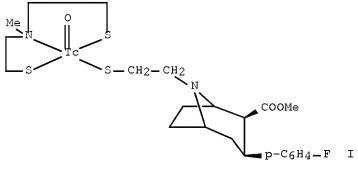
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6241963	B1	20010605	US 1996-649782	19960517 <--
CA 2233173	A1	19970424	CA 1996-2233173	19961021 <--
CA 2233173	C	20060404		
WO 9714445	A1	19970424	WO 1996-US16908	19961021 <--

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG

AU 9711566	A	19970507	AU 1997-11566	19961021 <--
AU 716235	B2	20000224		
EP 929319	A1	19990721	EP 1996-942721	19961021 <--
EP 929319	B1	20040922		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11514368	T	19991207	JP 1996-516091	19961021 <--
AT 276770	T	20041015	AT 1996-942721	19961021 <--
ES 2227621	T3	20050401	ES 1996-942721	19961021 <--
US 5980860	A	19991109	US 1998-116215	19980716 <--
PRIORITY APPLN. INFO.:			US 1995-545327	B2 19951019 <--
			US 1996-649782	A 19960517 <--
			WO 1996-US16908	W 19961021 <--

OTHER SOURCE(S): MARPAT 135:28327

GI



I

AB This invention presents a series novel tropane-based derivs. complexed with either Tc or Re that are specific for central nervous system receptors, in particular, dopamine or serotonin receptors. The compds. of the invention have utility, inter alia, as imaging agents for CNS receptors. Methods of using these novel compds. as imaging agents are presented, as are intermediates and methods for making these novel compds. For example, the 99Tc complex I was prepared from HSCH2CH2NMeCH2CH2SH and the resp. tropane derivative and its partition coefficient, brain uptake and stratum/cerebellum ratios were determined

IT 190022-00-5P

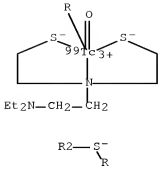
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(metastable; preparation and biodistribution studies as imaging agents)

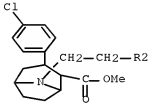
RN 190022-00-5 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][methyl (1R,2S,3S,5S)-3-(4-chlorophenyl)-8-[2-(mercapto-κS)ethyl]-8-azabicyclo[3.2.1]octane-2-carboxylato]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:186980 HCAPLUS Full-text
DOCUMENT NUMBER: 134:375325
TITLE: Reactivity of 99mTc(V) "3+1" mixed-ligand complexes towards glutathione
AUTHOR(S): Gupta, A.; Seifert, S.; Syhre, R.; Scheunemann, M.; Brust, P.; Johannsen, B.
CORPORATE SOURCE: Forschungszentrum Rossendorf, Institut fur Bioanorganische und Radiopharmazeutische Chemie, Dresden, D-01314, Germany
SOURCE: Radiochimica Acta (2001), 89(1), 43-49
CODEN: RAACAP; ISSN: 0033-8230
PUBLISHER: R. Oldenbourg Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:375325

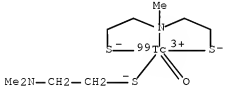
AB The stability and reactivity of mixed-ligand 99mTc complexes [99mTcOL1L2], where L1H2 is either an N-substituted bis(2-mercaptoethyl)amine [SNMeS] or 3-thiapentane-1,5-dithiol [SSS] and L2H is a monodentate thiol [RS], were studied. The complexes undergo transchelation reactions with glutathione and other SH-group containing blood constituents. The reactions are reversible and can be inhibited by addition of di-Et maleate. Challenge expts. were performed with a broad set of 99mTc mixed-ligand complexes to study the

influence of both the tridentate ligand and the monodentate ligand on the stability of this type of complex. The occurrence of ligand exchange reactions with glutathione depends on the donor set of the tridentate ligands as well as the structure of the monodentate ligands. Especially the stability of complexes containing a monodentate ligand with an amine N in the side chain can be increased by lengthening the C chain between the sulfhydryl group and the N. Thus, it might be possible to improve their in-vivo performance.

IT 178443-28-2P 202717-96-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and stability toward reaction with glutathione)

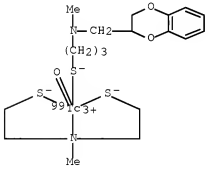
RN 178443-28-2 HCAPLUS

CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 202717-96-2 HCAPLUS

CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:101702 HCAPLUS Full-text

DOCUMENT NUMBER: 134:289479

TITLE: Synthesis, characterization and biological evaluation

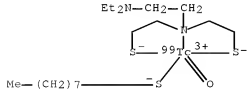
	of a novel "3 + 1" mixed ligand 99mTc complex having an aliphatic thiol as coligand
AUTHOR(S):	Rey, A.; Papadopoulos, M.; Leon, E.; Mallo, L.; Pirmettis, Y.; Manta, E.; Raptopoulou, C.; Chiotellis, E.; Leon, A.
CORPORATE SOURCE:	Catedra de Radioquimica y Catedra de Quimica Farmaceutica, Facultad de Quimica, Montevideo, 1157, Urug.
SOURCE:	Applied Radiation and Isotopes (2001), 54(3), 429-434 CODEN: ARISEF; ISSN: 0969-8043
PUBLISHER:	Elsevier Science Ltd.
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 134:289479

AB A novel "3 + 1" mixed ligand 99mTc complex with N,N-bis(2-mercaptoethyl)-N',N'-diethylethylenediamine as ligand and 1-octanethiol as coligand was prepared and evaluated as potential brain radiopharmaceutical. Preparation at tracer level was accomplished by substitution, using 99mTc-glucoheptonate as precursor and a coligand/ligand ratio of 5. Under these conditions the labeling yield was over 80% and a major product with radiochem. purity >80% was isolated by HPLC methods and used for biol. evaluation. Chemical characterization at carrier level was developed using the corresponding rhenium and 99gTc complexes. Results were consistent with the expected "3 + 1" structure and x-ray diffraction study of the rhenium complex demonstrated that the complex adopted a distorted trigonal bipyramidal geometry. All sulfur atoms underwent ionization giving a neutral compound Biodistribution in mice demonstrated early brain uptake, fast blood clearance and excretion through hepatobiliary system. Although brain/blood ratio increased significantly with time, this novel 99mTc complex did not exhibit ideal properties as brain perfusion radiopharmaceutical since brain uptake was too low.

IT 333404-59-4P
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and biol. evaluation of technetium bis(mercaptoethyl)diethylethylenediamine octanethiolate oxo "3 + 1" mixed ligand complex as brain perfusion radiopharmaceutical)

RN 333404-59-4 HCAPLUS

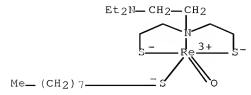
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1-octanethiolato)oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



IT 333404-55-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure)

RN 333404-55-0 HCAPLUS

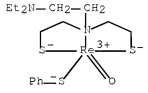
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1-octanethiolato)oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



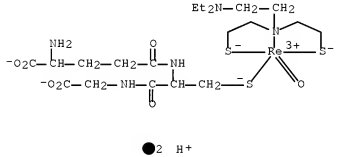
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:607688 HCAPLUS Full-text
DOCUMENT NUMBER: 133:316801
TITLE: Glutathione Interaction with SNS/S Mixed-Ligand Complexes of Oxorhenium(V): Kinetic Aspects and Characterization of the Products
AUTHOR(S): Nock, Berthold; Maina, Theodosia; Tsortos, Achilleas; Pelecanou, Maria; Raptopoulou, Catherine P.; Papadopoulos, Minas; Pietzsch, Hans-Juergen; Stassinopoulou, Chariklia I.; Terzis, Aris; Spies, Hartmut; Nounesis, Georgios; Chiotellis, Efstratios
CORPORATE SOURCE: Institute of RadioisotopesRadiodiagnostic Products, National Centre for Scientific Research Demokritos, Athens, 15310, Greece
SOURCE: Inorganic Chemistry (2000), 39(20), 4433-4441
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oxorhenium(V) SNS/S mixed-ligand complexes [ReO(Ln/L)] carrying different types of tridentate ligands (Ln) and the same monodentate coligand (L) [L = C6H5S, L1 = C2H5N(CH2CH2S)2 (1), L2 = Et2NCH2CH2N(CH2CH2S)2 (2), L3 = C2H5SCH2CH2N(CH2CH2S)2 (3), and L4 = 2,6-(SCH2)2NC5H3 (4)] were synthesized and characterized by spectroscopic methods and elemental analyses. X-ray structure determination was performed for complexes 3 and 4. 3 Adopts the expected distorted trigonal bipyramidal geometry around the metal in a syn configuration, while 4, due to the aromatic character of the N of the SNS donor-atom set, exhibits a distorted square pyramidal geometry. Interaction of 1-4 with glutathione (GSH) was studied by HPLC, revealing the rapid formation of the resp. daughter complexes 5-8 ReO(Ln)(GS), wherein GS is substituted for L. 5-8 Were characterized by ES-MS and 2-dimensional NMR spectroscopy. Kinetic aspects of the interaction of 1-3 with GSH were studied by isothermal titration microcalorimetry providing direct measurements of the interaction rate consts. and of the total enthalpy change. The reaction of complex 1 exhibits the slowest rate and that of complex 2 the fastest. This is in agreement with previously reported trends for analogous 99mTc complexes.
IT 178476-52-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(kinetics and enthalpy of coordinative substitution reaction with

glutathione)
RN 178476-52-3 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



IT 224432-57-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from coordinative substitution of glutathione with Ph thiol analog)
RN 224432-57-9 HCAPLUS
CN Rhenate(2-), [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][L-γ-glutamyl-L-cysteinyl-κS-glycinato(3-)]oxo-, dihydrogen, (TB-5-14)- (9CI) (CA INDEX NAME)



2 H+

OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:584353 HCAPLUS Full-text
DOCUMENT NUMBER: 133:278069
TITLE: Permeation studies in vitro and in vivo of potential radiopharmaceuticals with affinity to neuro receptors
AUTHOR(S): Friebe, Matthias; Suda, Kayoshi; Spies, Hartmut; Syhre, Rosmarie; Berger, Ralf; Johannsen, Bernd; Chiotellis, Efstratios; Kramer, Stefanie D.; Wunderli-Allenspach, Heidi
CORPORATE SOURCE: Department of Pharmacy, Biopharmacy, Swiss Federal Institute of Technology, Zurich, Switz.
SOURCE: Pharmaceutical Research (2000), 17(6), 754-760
CODEN: PHREEB; ISSN: 0724-8741

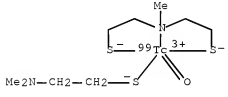
PUBLISHER: Kluwer Academic/Plenum Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Purpose: To check the influence of structural characteristics on their permeation through the blood-brain barrier (BBB), a set of radioactive [99mTc]chelates bearing amine groups was synthesized and tested in vitro as well as in vivo. Methods: Compds. with different log P and pKa values were obtained by complex forming reactions of [99mTc]pertechnetate with varying substituents. Transport was studied in rats and mice, as well as in an ECV304 cell culture model. Results: In vitro higher permeation was found for compds. with electron attracting substituents in β-position to the amine group (pKa values 7.4 to 8.3) than for those with more basic amine groups (pKa values > 8.9) even for similar log DpH 7.4. In vivo brain uptake between 0.8 and 4.8% of the injected dose (ID) per organ was found for the former, whereas < 0.4% ID were present for the latter. Conclusions: Three structurally diverse classes of [99mTc]chelates showed distinct patterns with regard to brain uptake in vivo and BBB permeability in vitro which could not be predicted by their lipophilicity alone. The close correlation between the data from rats and mice and those obtained with cell cultures render the ECV304 cells an attractive model for the screening of new compds.

IT 178443-28-2P 178443-29-3P 178443-31-7P
190580-27-9P 190580-28-0P 190580-29-1P
190580-32-6P 190580-34-8P 205577-85-1P
205578-08-1P 205578-09-2P 205578-10-5P
206761-53-7P 206761-54-8P 206761-55-9P
300343-61-7P 300343-62-8P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(blood-brain barrier permeation study of potential radiopharmaceuticals with affinity to neuro-receptors)

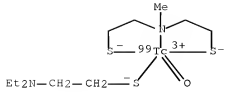
RN 178443-28-2 HCAPLUS

CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

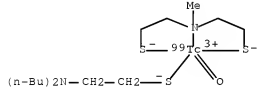


RN 178443-29-3 HCAPLUS

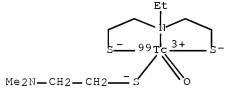
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



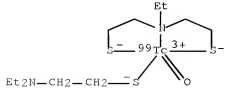
RN 178443-31-7 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190580-27-9 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

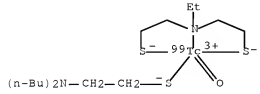


RN 190580-28-0 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

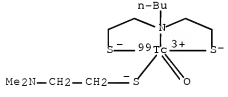


RN 190580-29-1 HCAPLUS

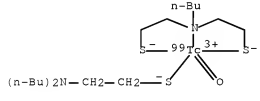
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



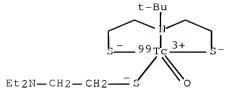
RN 190580-32-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



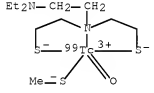
RN 190580-34-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



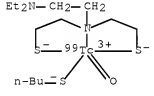
RN 205577-85-1 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



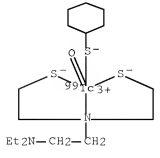
RN 205578-08-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](methanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



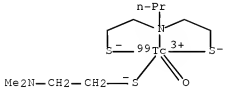
RN 205578-09-2 HCAPLUS
CN Technetium-99Tc, (1-butanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



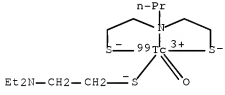
RN 205578-10-5 HCAPLUS
CN Technetium-99Tc, (cyclohexanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



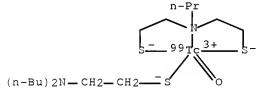
RN 206761-53-7 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



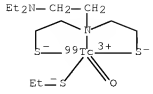
RN 206761-54-8 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



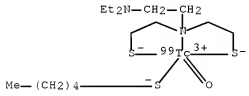
RN 206761-55-9 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 300343-61-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](ethanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 300343-62-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo(1-pentanethiolato)-, (SP-5-31)- (9CI) (CA INDEX NAME)

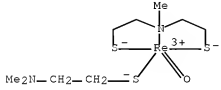


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

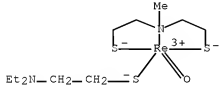
L13 ANSWER 9 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:464506 HCAPLUS Full-text
DOCUMENT NUMBER: 133:290233
TITLE: Neutral '3 + 1' mixed-ligand oxorhenium(V) complexes with tridentate [S,N,S] chelates and aminoalkanethiols: synthesis, characterization and structure determination
AUTHOR(S): Friebe, Matthias; Spies, Hartmut; Seichter, Wilhelm; Leibnitz, Peter; Johannsen, Bernd
CORPORATE SOURCE: Forschungszentrum Rossendorf, Institut fur Bioanorganische und Radiopharmazeutische Chemie, Dresden, D-01314, Germany
SOURCE: Dalton (2000), (14), 2471-2475
CODEN: DALTFG; ISSN: 1470-479X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB '3 + 1' Oxorhenium(V) complexes [ReO(SCH2CH2N(R')CH2CH2S)(SR)] (R' = Me, Et, Pr or Bu; SR = aminoalkanethiolate) were synthesized by ligand exchange at trans-trichloromonooxobis(triphenylphosphine)rhenium(V) with a mixture of HSCH2CH2N(R')CH2CH2SH and RSH in alkaline methanolic solution The complexes were purified by column chromatog. and characterized by elemental anal., mass and IR spectroscopy and for selected compds. by 1H NMR spectroscopy. The structures of three complexes were determined by x-ray diffraction anal. and revealed a change in the coordination geometry from square pyramidal to trigonal bipyramidal, depending on the chelating (SN(R')S) moiety. The alkyl group (R') is arranged syn to the oxorhenium group.
IT 190588-01-3P 190588-02-4P 190588-03-5P

190588-06-8P 190588-07-9P 190588-08-0P
190588-11-5P 190588-12-6P 190588-13-7P
206761-58-2P 206761-59-3P 206761-60-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

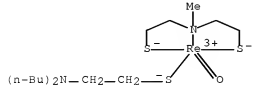
RN 190588-01-3 HCAPLUS
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



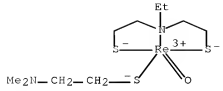
RN 190588-02-4 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



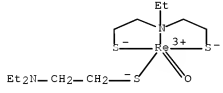
RN 190588-03-5 HCAPLUS
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



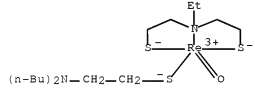
RN 190588-06-8 HCAPLUS
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



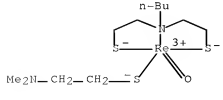
RN 190588-07-9 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-08-0 HCAPLUS
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

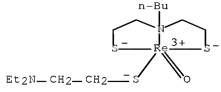


RN 190588-11-5 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



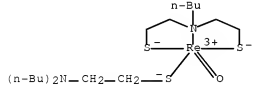
RN 190588-12-6 HCAPLUS

CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



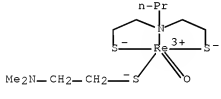
RN 190588-13-7 HCAPLUS

CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



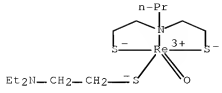
RN 206761-58-2 HCAPLUS

CN Rhenium, [2-(dimethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



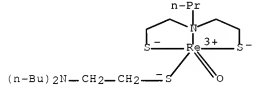
RN 206761-59-3 HCAPLUS

CN Rhenium, [2-(diethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 206761-60-6 HCAPLUS

CN Rhenium, [2-(dibutylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:410597 HCAPLUS Full-text

DOCUMENT NUMBER: 133:171463

TITLE: '3+1' Mixed-Ligand Oxotechnetium(V) Complexes with Affinity for Melanoma: Synthesis and Evaluation in Vitro and in Vivo

AUTHOR(S): Friebe, Matthias; Mahmood, Ashfaq; Spies, Hartmut; Berger, Ralf; Johannsen, Bernd; Mohammed, Ashour; Eisenhut, Michael; Bolzati, Cristina; Davison, Alan; Jones, Alun G.

CORPORATE SOURCE: Department of Radiology, Harvard Medical School and Brigham and Women's Hospital, Boston, MA, 02115, USA

SOURCE: Journal of Medicinal Chemistry (2000), 43(14), 2745-2752
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

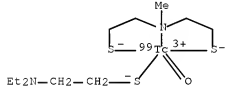
AB '3+1' Mixed-ligand [99mTc]oxotechnetium complexes with affinity for melanoma were synthesized in a 1-pot reaction. Complexation of 99mTc with a mixture of N-R(3-azapentane-1,5-dithiol) [R = Me, Pr, Bn, Et2N(CH2)2] and N-(2-dialkylamino)ethanethiol [alkyl = X = Et, Bu, morpholinyl] using Sn2+ as the reducing agent gave '3+1' mixed-ligand 99mTc complexes [TcO(SN(R)S)(SNX2)] in high radiochem. yield (60-98%). In vitro uptake studies in B16 murine melanoma cells indicated a moderate tumor-cell accumulation (40%) of compound 1 [R = Me, X = Et] and a higher accumulation (69%) of compound 2 [R = Me, X = Bu] after a 60-min incubation. In vivo evaluation of compds. 1-6 in the C57B16/B16 mouse melanoma model demonstrated tumor localization. Compound 2

displayed the highest accumulation with up to 5% ID/g at 60 min after injection. In vivo, 2 also showed a low blood-pool activity and high melanoma/spleen (4.3) and melanoma/lung (1.9) ratios at 1 h. Probably small 99mTc complexes are useful as potential melanoma-imaging agents.

IT 178443-29-3P 178443-31-7P 205578-08-1P
206761-55-9P 287962-60-1P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation, affinity for melanoma, lipophilicity and pKa of)

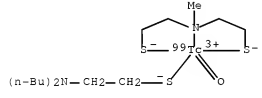
RN 178443-29-3 HCAPLUS

CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



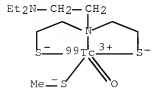
RN 178443-31-7 HCAPLUS

CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



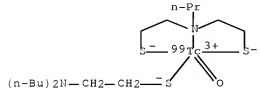
RN 205578-08-1 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](methanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

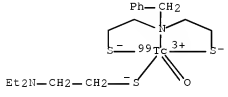


RN 206761-55-9 HCAPLUS

CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 287962-60-1 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS]oxo[[2,2'-[(phenylmethyl)imino-κN]bis[ethanethiolato-κS]](2-)]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

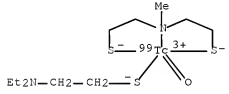
L13 ANSWER 11 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:289834 HCAPLUS Full-text
DOCUMENT NUMBER: 134:33494
TITLE: Basicity of amine group containing "3+1" Re complexes studied by HPLC
AUTHOR(S): Berger, R.; Friebe, M.; Glaser, M.; Pietzsch, H.-J.; Maina, T.; Chiotellis, E.; Spies, H.
CORPORATE SOURCE: Inst. of Radioisotopes-Radiodiagnostic Products, Natl. Centre for Scientific Research "Demokritos", Athens, Greece
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-283, 97-99 CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report
LANGUAGE: English
AB Rhenium or technetium oxo complexes with one tridentate and one thiol ligand containing the amino group in different positions were studied by HPLC. The acid-base properties of these complexes were derived from turning points in lipophilicity/pH profiles of the chromatograms. The nature and position of the amino group in Re/Tc complexes are tools for directing the basicity either to bring about a small decrease in basicity compared to the free amine ligand or to produce species of drastically reduced basicity. The basicity of a tracer is an important property that governs its in vivo transport, so a

knowledge of structure-basicity relationships is essential in radiotracer design.

IT 178443-29-3 178476-50-1 190580-28-0
190580-33-7 190588-02-4 190588-07-9
190588-12-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(HPLC estimation of acid-base properties of rhenium or technetium complexes with amine ligands)

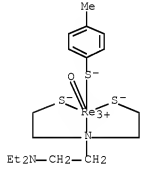
RN 178443-29-3 HCAPLUS

CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



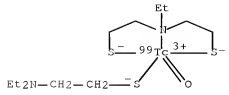
RN 178476-50-1 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

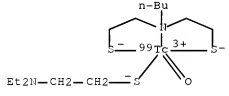


RN 190580-28-0 HCAPLUS

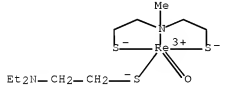
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



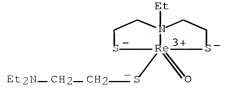
RN 190580-33-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190588-02-4 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

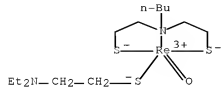


RN 190588-07-9 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-12-6 HCAPLUS

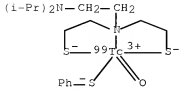
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



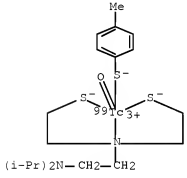
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:232069 HCAPLUS Full-text
DOCUMENT NUMBER: 132:342352
TITLE: Oxorhenium and oxotechnetium [SNS/S] mixed ligand complexes having a pendant diisopropylaminoethyl-group. Synthesis, characterization and biodistribution studies
AUTHOR(S): Rey, A.; Papadopoulos, M.; Mallo, L.; Pirmettis, I.; Leon, E.; Raptopoulou, C.; Manta, E.; Chiotellis, E.; Leon, A.
CORPORATE SOURCE: Facultad de Quimica, Catedras de Radioquimica y Quimica Farmaceutica, Montevideo, Urug.
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2000), 43(4), 347-358
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel SNS tridentate ligand, the N,N-bis(2-mercaptoethyl)-N',N'-diisopropylethylenediamine (H2L) was synthesized and ReOL(SC6H4R-4) (R = H, Me, Cl) and 99mTcOL(SC6H4R-4) were prepared and characterized. ReOL(SC6H4R-4) were prepared from ReO(PPh3)2Cl3 and H2L and HSC6H4R-4. Characterization was performed by HPLC anal., UV-visible and IR spectra, elemental anal. and x-ray diffraction. The complexes adopted a distorted trigonal bipyramidal geometry. Consequently 99mTc complexes were also prepared and evaluated in mice as potential brain imaging agents. Labeling was performed by substitution using 99mTc-glucoheptonate as precursor. The labeling yield was over 85% and the radiochem. purity of the complexes over 90%. Biodistribution in mice demonstrated high uptake and retention in brain. However comparison with previously reported mixed ligand complexes showed that the incorporation of the diisopropylaminoethyl group in the SNS/S backbone is not enhancing the biol. characteristics of this type of complexes.
IT 267400-41-9P 267400-42-0P 267400-43-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biodistribution study for imaging agents)
RN 267400-41-9 HCAPLUS
CN Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-[bis(1-

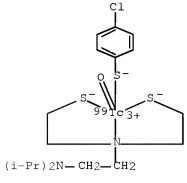
methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-
)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



RN 267400-42-0 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-,
(SP-5-34)- (9CI) (CA INDEX NAME)

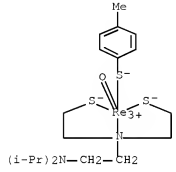


RN 267400-43-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)](4-chlorobenzenethiolato-
κS)oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)

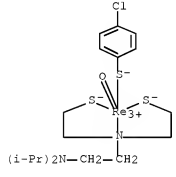


IT 267400-38-4P 267400-39-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

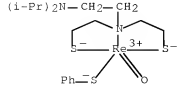
RN 267400-38-4 HCAPLUS
CN Rhenium, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-23)- (9CI) (CA INDEX NAME)



RN 267400-39-5 HCAPLUS
CN Rhenium, [[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-chlorobenzenethiolato-κS)oxo-, (TB-5-23)- (9CI) (CA INDEX NAME)



IT 267400-37-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 267400-37-3 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[2-[bis(1-methylethyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-23)- (9CI) (CA INDEX NAME)



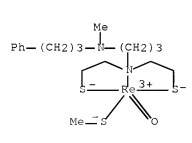
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:64365 HCAPLUS Full-text
DOCUMENT NUMBER: 132:242376
TITLE: Miscellaneous results of determining the partition coefficients and ionization constants for rhenium and technetium coordination compounds by using HPLC
AUTHOR(S): Berger, R.; Wust, F.; Zablotskaya, A.; Friebe, M.; Pietzsch, H.-J.; Scheunemann, M.; Reigys, M.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Latvian Institute of Organic Chemistry, Riga, Latvia
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-270, 202-209
CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report
LANGUAGE: German

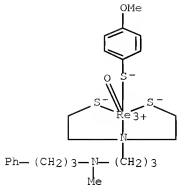
AB Using PRP-1 column and 3:1 acetonitrile-buffer eluent, HPLC behavior of the title compds. was studied. Effects of protonable nitrogen atoms, ligand-exchange activities, nos. of carbon atoms in side chains, hydroxyl or silyl substitution in coordinated ligands are discussed. The corresponding lipophilicity values and ionization consts. are tabulated.

IT 178443-47-5 178443-48-6 191022-08-9
202717-96-2 202717-97-3 202717-98-4
205577-78-2 207567-05-3 261961-24-4
261961-30-2 261961-31-3 261961-32-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(HPLC study of lipophilicity and ionization of rhenium and technetium coordination compds.)

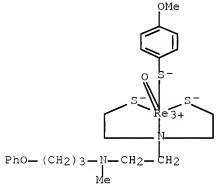
RN 178443-47-5 HCAPLUS
CN Rhenium, (methanethiolato)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



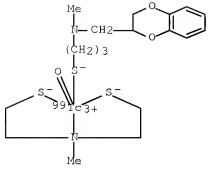
RN 178443-48-6 HCAPLUS
CN Rhenium, (4-methoxybenzenethiolato-κS)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



RN 191022-08-9 HCAPLUS
CN Rhenium, (4-methoxybenzenethiolato-κS)[[2,2'-[[2-[methyl(3-phenoxypropyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)

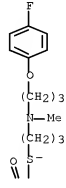


RN 202717-96-2 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

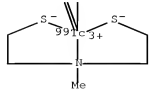


RN 202717-97-3 HCAPLUS
CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A

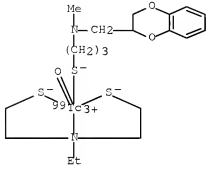


PAGE 2-A



RN 202717-98-4 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-

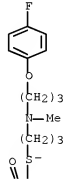
yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



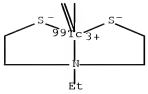
RN 205577-78-2 HCAPLUS

CN Technetium-99Tc, [[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)][3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

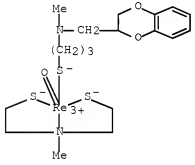
PAGE 1-A



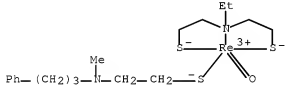
PAGE 2-A



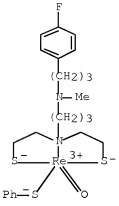
RN 207567-05-3 HCAPLUS
CN Rhenium, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



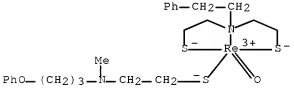
RN 261961-24-4 HCAPLUS
CN Rhenium, [[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)][2-[methyl(3-phenylpropyl)amino]ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



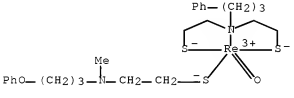
RN 261961-30-2 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[3-[[3-(4-fluorophenyl)propyl]methylamino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



RN 261961-31-3 HCAPLUS
CN Rhenium, [2-[methyl(3-phenoxypropyl)amino]ethanethiolato-κS]oxo[[2,2'-[(2-phenylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 261961-32-4 HCAPLUS
CN Rhenium, [2-[methyl(3-phenoxypropyl)amino]ethanethiolato-κS]oxo[[2,2'-[(3-phenylpropyl)imino-κN]bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

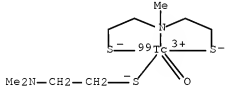
L13 ANSWER 14 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:64359 HCAPLUS Full-text
DOCUMENT NUMBER: 132:302876
TITLE: Reactivity of "3+1" 99mTc complexes to proteins
AUTHOR(S): Seifert, S.; Gupta, A.; Syhre, R.

CORPORATE SOURCE: Germany
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-270, 181-184
CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report
LANGUAGE: English

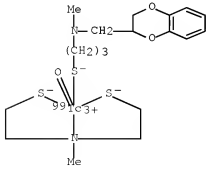
AB Possibilities of labeling SH-containing components of the blood with "3+1" 99mTc complexes were investigated. Some of the complexes reacted with plasma and blood proteins which replaced the monodentate ligand in the complexes. Only the monothiol ligand was exchanged. All "3+1" complexes investigated were metabolized in the whole blood in vitro and in vivo into glutathione (GSH)-containing complexes. While the [99mTcO(SNMeS/GS)] complex was stable in rat and human plasma, the more unstable [99mTcO(SSS/GS)] complex with dimethylcysteamine reacted with albumin and globulin.

IT 178443-28-2 265642-06-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); BIOL (Biological study); PROC (Process)
(reactivity of "3+1" 99mTc complexes to proteins)

RN 178443-28-2 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

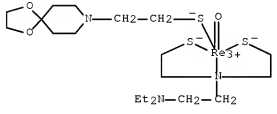


RN 265642-06-6 HCAPLUS
CN Technetium-99Tc, [3-[[[(2S)-2,3-dihydro-1,4-benzodioxin-2-yl]methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 15 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:64357 HCAPLUS Full-text
DOCUMENT NUMBER: 132:273260
TITLE: Identification of the transchelation product of "3+1" mixed-ligand technetium and rhenium complexes with glutathione
AUTHOR(S): Gupta, A.; Seifert, S.; Syhre, R.; Johannsen, B.
CORPORATE SOURCE: Germany
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-270, 173-176
CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report
LANGUAGE: German
AB Rhenium and technetium-99 complexes with glutathione and bis(2-ethanethiol)sulfide and bis(2-ethanethiol)methylamine were prepared and compared with the products resulting from GSH challenge expts.
IT 218788-15-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of rhenium bis(2-ethanethiol)sulfide and bis(2-ethanethiol)methylamine glutathione complexes)
RN 218788-15-9 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1,4-dioxa-8-azaspiro[4.5]decane-8-ethanethiolato-κS8)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 16 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:64356 HCAPLUS Full-text
DOCUMENT NUMBER: 132:287865
TITLE: Challenge experiments with "3+1" mixed-ligand 99mTc complexes and glutathione: influence of structural parameters on the complex stability
AUTHOR(S): Gupta, A.; Seifert, S.; Syhre, R.; Johannsen, B.
CORPORATE SOURCE: Germany
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-270, 167-172
CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report

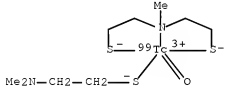
LANGUAGE: German

AB 99Tc(L)(RS) (L = S(CH2)2E(CH2)2S, E = S, NMe; R = aryl or N containing alkyl groups) were prepared and coordinative substitution reactions with glutathione (GSH) were studied. Kinetic studies reveal that the complexes with E = NMe tridentate ligand form more stable trans-chelates with glutathione and a N atom in the monodentate ligand has a destabilizing effect on GSH complex formation.

IT 178443-28-2P 202717-96-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coordinative substitution reaction with glutathione)

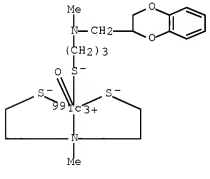
RN 178443-28-2 HCAPLUS

CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 202717-96-2 HCAPLUS

CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 17 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:42813 HCAPLUS Full-text

DOCUMENT NUMBER: 132:188928

TITLE: A "preformed chelate approach" model for coupling

amine-modified rhenium and technetium "3+1" mixed ligand complexes to carboxylate residues Crystal structure of ReO[CH3SCH2CH2N(CH2CH2S)2][p-SC6H4NH2] and ReO[CH3SCH2CH2N(CH2CH2S)2][p-SC6H4NHCOC6H5]

AUTHOR(S): Maina, Theodosia; Tsoukalas, Charalambos; Patsis, Georgios; Pirmettis, Ioannis; Nock, Berthold; Papadopoulos, Minas; Raptopoulou, Catherine; Terzis, Aris; Chiotellis, Efstratios

CORPORATE SOURCE: Institute of Radioisotopes-Radiodiagnostic Products, NCSR "Demokritos", Athens, Greece

SOURCE: Polyhedron (1999), 18(26), 3545-3552
CODEN: PLYHDE; ISSN: 0277-5387

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

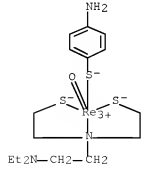
LANGUAGE: English

AB Selected '3+1' mixed ligand oxorhenium and oxotechnetium complexes containing the SNS/S donor atom set were modified by introduction of a bifunctional amine anchor on the p-position of the thiophenolato monodentate ligand. A representative series of complexes containing several tridentate ligands was prepared both at macromolar (Re complexes) and nanomolar (99mTc complexes) amts. Coupling of these complexes to activated carboxylate groups was performed according to the preformed chelate approach using benzoyl chloride as a model mol. Coupling yields were high both at nanomolar and millimolar metal concentration, as revealed by HPLC anal. of 99mTc and Re species adopting parallel radiometric and photometric detection modes. All Re compds. were characterized by classical anal. methods. The structures of representative parent ReO[CH3SCH2CH2N(CH2CH2S)2][p-SC6H4NH2] and daughter ReO[CH3SCH2CH2N(CH2CH2S)2][p-SC6H4NHCOC6H5] complexes were solved by x-ray crystallog. Both compds. adopt a distorted trigonal bipyramidal geometry around Re, wherein the oxo group and the S atoms of the SNS ligand occupy the equatorial plane and the N atom and the S of the monothiol are located at the apical positions trans to each other.

IT 178476-48-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling to benzoyl chloride)

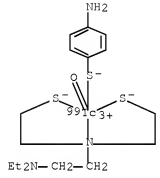
RN 178476-48-7 HCAPLUS

CN Rhenium, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

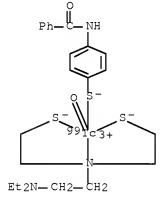


IT 221100-24-9
RL: RCT (Reactant); RACT (Reactant or reagent)

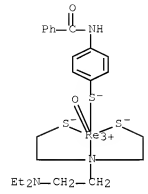
(metastable; coupling to benzoyl chloride)
RN 221100-24-9 HCAPLUS
CN Technetium-99Tc, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



IT 259260-98-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(metastable; preparation as model for coupling of amine-modified technetium-99m complex to carboxylate residues)
RN 259260-98-5 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][N-[4-(mercapto-κS)phenyl]benzamidato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



IT 259260-92-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation as model for coupling of amine-modified rhenium complex to carboxylate residues)
RN 259260-92-9 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][N-[4-(mercapto-κS)phenyl]benzamidato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



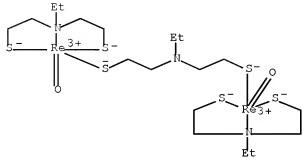
OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 18 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:739403 HCAPLUS Full-text
DOCUMENT NUMBER: 132:101928
TITLE: Study on the formation of mixed ligand oxorhenium and oxotechnetium complexes (SNS/S combination)
AUTHOR(S): Papadopoulos, M.; Pirmettis, I.; Tsoukalas, C.; Nock, B.; Maina, T.; Raptopoulou, C. P.; Pietzsch, H.-J.; Friebe, M.; Spies, H.; Johannsen, B.; Chiotellis, E.
CORPORATE SOURCE: NCSR 'Demokritos', Institute of Radioisotopes and Radiodiagnostic Products, Athens, 153 10, Greece
SOURCE: Inorganica Chimica Acta (1999), 295(1), 1-8
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Theor., several complexes can be formed during the reaction between the tridentate aminedithiol ligand EtN(CH2CH2SH)2, L1H2, the monodentate thiol p-ClC6H4SH, L2H, and ReVOCl3(PPh3)2. Three main possibilities are: (i) neutral mixed ligand complexes ReOL1L2, the syn isomer (complex 1) and the anti isomer (complex 2); (ii) binuclear complex of the tridentate ligand, (ReO)2(L1)3 (complex 3) and (iii) anionic complex of the monothiol [ReO(L2)4]- (complex 4). When a mixture of L1H2/L2H, 1/1 ratio, is applied, the major product of the reaction is the syn isomer 1. A small amount of the anti isomer 2 is also isolated (yield <2%) while none of the complexes 3 and 4 are formed under the above reaction conditions. The oxorhenium complexes 3 and 4 were synthesized by the reaction of L1H2 or L2H resp. with the precursor ReOCl3(PPh3)2. The crystal structures of 1, 3, and 4 are determined by x-ray crystallog. The corresponding 99mTc complexes were prepared by exchange reaction using 99mTc-glucoheptonate as precursor. Similarly the major reaction product is the syn isomer, complex 1', while none of the other complexes are formed during the reaction at tracer level. Simultaneous action of a tridentate SNS ligand and a monodentate thiol in equimolar quantities on ReVOCl3(PPh3)2 or 99mTc-glucoheptonate leads to a single rhenium or technetium-99m species, the syn MOL1L2.

IT 254443-02-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

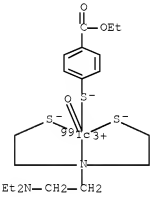
(preparation and crystal and mol. structure)
RN 254443-02-2 HCAPLUS
CN Rhenium, [μ-[[2,2'-(ethylimino)bis[ethanethiolato-κS]](2-)]]bis[[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]dioxodi-, stereoisomer (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 19 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:410443 HCAPLUS Full-text
DOCUMENT NUMBER: 131:211022
TITLE: The potential role of intracerebral glutathione in the retention of a representative 99mTc SNS/S mixed ligand complex in mice brain
AUTHOR(S): Nock, B. A.; Maina, T.; Pirmettis, I.; Papadopoulos, M.; Tsoukalas, C.; Chiotellis, E.
CORPORATE SOURCE: Institute of Radioisotopes - Radiodiagnostic Products, NCSR "Demokritos", Athens, 15310, Greece
SOURCE: Czechoslovak Journal of Physics (1999), 49(Suppl. 1, Pt. 2, 13th Radiochemical Conference, 1998), 873-877
CODEN: CZYPAO; ISSN: 0011-4626
PUBLISHER: Institute of Physics, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis, radiochem. and biodistribution in mice of 99mTcO[[(CH3CH2)2NCH2CH2N(CH2CH2S)2] (p-SPh-COOCH2CH3)], I, are reported herein. Complex I forms by binding of (CH3CH2)2NCH2CH2N(CH2CH2SH)2 and p-HSPhCOOCH2CH3 ligands to reduced 99mTc using glucoheptonate (GH) as transfer ligand. Corroboration of structure with an authentic 99gTc sample is achieved by reverse phase high pressure liquid chromatog. (RP-HPLC) adopting parallel radiometric and photometric detection modes. By incubation at 37℃ with glutathione (GSH) in aqueous medium I transforms to an hydrophilic compound, as shown by HPLC. Tissue distribution expts. reveal high uptake and retention of I in mice brain.
IT 231633-15-1P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of and role of glutathione in retention of99mTc SNS/S mixed

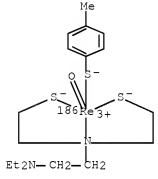
ligand complex in brain)
RN 231633-15-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][ethyl 4-(mercapto-κS)benzoato]oxo-, stereoisomer (9CI) (CA INDEX NAME)



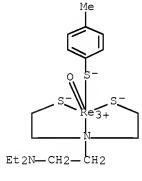
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 20 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:319995 HCAPLUS Full-text
DOCUMENT NUMBER: 131:27082
TITLE: Structural studies of ReO(V) mixed ligand [SNS][Cl] and [SNS][S] complexes
AUTHOR(S): Pelecanou, M.; Pirmettis, I. C.; Papadopoulos, M. S.; Raptopoulou, C. P.; Terzis, A.; Chiotellis, E.; Stassinopoulou, C. I.
CORPORATE SOURCE: Institute of Biology, NCSR Demokritos, Athens, GR-153 10, Greece
SOURCE: Inorganica Chimica Acta (1999), 287(2), 142-151
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis, characterization and spectroscopic properties of four oxorhenium complexes, ReO[C2H5SCH2CH2N(CH2CH2S)2]Cl (1), ReO[C2H5SCH2CH2N(CH2CH2S)2][p-CH3OC6H4S] (2), ReO[Et2NCH2CH2N(CH2CH2S)2][p-CH3C6H4S] (3), and ReO[C5H10NCH2CH2N(CH2CMe2S)2][C6H5CH2S] (4) are reported. These neutral and lipophilic complexes are designed according to the '3 + 1' mixed ligand concept. X-ray crystallog. studies show that the coordination geometry around Re is distorted trigonal bipyramidal in 2 and 3 and trigonally distorted square pyramidal in 4. Crystal data: 2, triclinic space group P.hivin.1, a 9.610(2), b 9.628(2), c 11.791(2) Å, α 108.307(8), β 67.735(6), γ 90.166(8)°, Z = 2; 3, monoclinic space group P21/c, a 13.188(1), b 7.542(1), c 21.193(1) Å, β 103.260(2)°, Z = 4; 4, monoclinic P21/c, a 16.720(6), b 11.013(3), c 16.747(5) Å, β 113.44(1)°, Z = 4. Complete assignments of 1H and 13C NMR resonances were made for all complexes and compared to those of analogous Tc complexes. ΔG≠. 3 Was also prepared at the tracer 186Re level.
IT 226545-19-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclic voltammetry)
RN 226545-19-3 HCAPLUS
CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



IT 178476-50-1P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation, crystal structure, cyclic voltammetry, and ligand conformational inversion)
RN 178476-50-1 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 21 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:259863 HCAPLUS Full-text
DOCUMENT NUMBER: 131:99320
TITLE: Characterization and preliminary evaluation of

ester-modified technetium-99m SNS/S mixed ligand complexes as potential brain perfusion agents

AUTHOR(S): Tsoukalas, C.; Papadopoulos, M. S.; Maina, T.; Pirmettis, I. C.; Nock, B. A.; Raptopoulou, C.; Terzis, A.; Chiotellis, E.

CORPORATE SOURCE: Institute of Radioisotopes, Radiodiagnostic Products, NCSR "Demokritos,", Athens, 153 10, Greece

SOURCE: Nuclear Medicine and Biology (1999), 26(3), 297-304
CODEN: NMBIEO; ISSN: 0969-8051

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

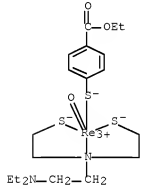
LANGUAGE: English

AB Two novel [99mTc](SNS/S) mixed ligand complexes carrying a pendant ester function on the monothiolate coligand were synthesized. The corresponding oxorhenium and [99gTc]oxotechnetium complexes prepared at the macroscopic level and chemical characterized were used for structure assignment of [99mTc](SNS/S) complexes prepared at the nanomolar level. Enzymic hydrolysis of the pendant ester group of [99mTc](SNS/S) mixed ligand complexes by esterase was investigated in vitro and compared with that of the Et cysteinate dimer, [99mTc]ECD. Preliminary biodistribution data in mice shows that the complexes are lipophilic and exhibit significant initial uptake in rodent brain.

IT 231633-07-1P 231633-11-7P 231633-15-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, characterization and brain uptake of ester-modified technetium-99m SNS/S mixed ligand complexes)

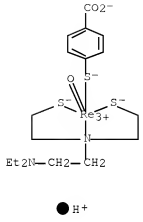
RN 231633-07-1 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][ethyl 4-(mercapto-κS)benzoato]oxo-, stereoisomer (9CI) (CA INDEX NAME)

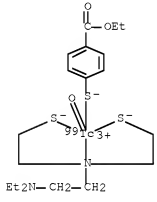


RN 231633-11-7 HCAPLUS

CN Rhenate(1-), [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(mercapto-κS)benzoato(2-)]oxo-, hydrogen, stereoisomer (9CI) (CA INDEX NAME)



RN 231633-15-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][ethyl 4-(mercapto-κS)benzoato]oxo-, stereoisomer (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 22 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:152815 HCAPLUS Full-text
DOCUMENT NUMBER: 130:334725
TITLE: Glutathione-Mediated Metabolism of Technetium-99m SNS/S Mixed Ligand Complexes: A Proposed Mechanism of Brain Retention
AUTHOR(S): Nock, Berthold A.; Maina, Theodosia; Yannoukakos, Drakoulis; Pirmettis, Ioannis C.; Papadopoulos, Minas S.; Chiotellis, Efstratios
CORPORATE SOURCE: Institute of Radioisotopes - Radiodiagnostic Products, NCSR Demokritos, Athens, 153 10, Greece
SOURCE: Journal of Medicinal Chemistry (1999), 42(6),

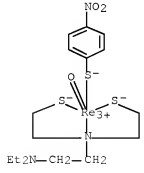
1066-1075
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two series of [99mTc](SNS/S) mixed ligand complexes each carrying the N-diethylaminoethyl or the N-ethyl-substituted bis(2-mercaptoethyl)amine ligand (SNS) are produced at tracer level using tin chloride as reductant and glucoheptonate as transfer ligand. The identity of [99mTc](SNS/S) complexes is established by high-performance liquid chromatog. (HPLC) comparison with authentic rhenium samples. The para substituent R on the phenylthiolate coligand (S) ranges from electron-donating (-NH2) to electron-withdrawing (-NO2) groups, to study complex stability against nucleophiles as a result of N- and R-substitution. The relative resistance of [99mTc](SNS/S) complexes against nucleophilic attack of glutathione (GSH), a native nucleophilic thiol of 2 mM intracerebral concentration, is investigated in vitro by HPLC. The reaction of [99mTc](SNS/S) complexes with GSH is reversible and advances via substitution of the monothiolate ligand by GS- and concomitant formation of the hydrophilic [99mTc](SNS/GS) daughter compound The N-diethylaminoethyl complexes are found to be more reactive against GSH as compared to the N-Et ones. Complex reactivity as a result of R-substitution follows the sequence -NO2 » -H > -NH2. These in vitro findings correlate well with in vivo distribution data in mice. Thus, brain retention parallels complex susceptibility to GSH attack. Furthermore, isolation of the hydrophilic [99mTc](SNS/GS) metabolite from biol. fluids and brain homogenates provides addnl. evidence that the brain retention mechanism of [99mTc](SNS/S) complexes is GSH-mediated.

IT 178476-56-7
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(glutathione-mediated metabolism and brain retention of technetium-99m mixed ligand complexes)

RN 178476-56-7 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-nitrobenzenethiolato-κS)oxo-, (TB-5-14)- (CA INDEX NAME)

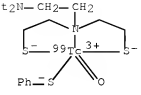


IT 174537-62-3P 221100-24-9P 224431-49-6P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(glutathione-mediated metabolism and brain retention of technetium-99m

mixed ligand complexes)

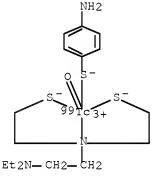
RN 174537-62-3 HCAPLUS

CN Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)



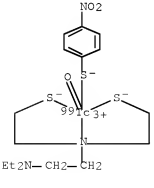
RN 221100-24-9 HCAPLUS

CN Technetium-99Tc, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

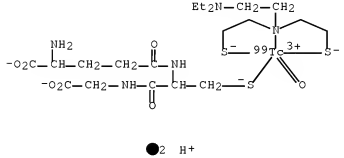


RN 224431-49-6 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-nitrobenzenethiolato-κS)oxo-, stereoisomer (CA INDEX NAME)

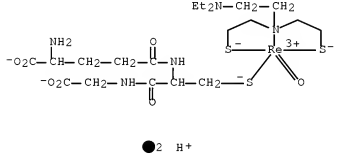


IT 224431-86-1 224432-57-9
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(glutathione-mediated metabolism and brain retention of technetium-99m mixed ligand complexes)
RN 224431-86-1 HCAPLUS
CN Technetate(2-)-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][L-γ-glutamyl-L-cysteinyl-κS-glycinato(3-)]oxo-, dihydrogen, (TB-5-14)- (9CI) (CA INDEX NAME)



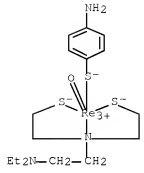
2 H+

RN 224432-57-9 HCAPLUS
CN Rhenate(2-), [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][L-γ-glutamyl-L-cysteinyl-κS-glycinato(3-)]oxo-, dihydrogen, (TB-5-14)- (9CI) (CA INDEX NAME)

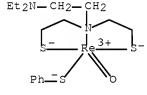


2 H+

IT 178476-48-7 178476-52-3
RL: PRP (Properties)
(glutathione-mediated metabolism and brain retention of technetium-99m mixed ligand complexes)
RN 178476-48-7 HCAPLUS
CN Rhenium, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-52-3 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 51 THERE ARE 51 CAPLUS RECORDS THAT CITE THIS RECORD (51 CITINGS)
REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 23 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:77968 HCAPLUS Full-text
DOCUMENT NUMBER: 130:231346
TITLE: Synthesis and characterization of five-coordinate rhenium(V) and technetium(V) mixed ligand bifunctional complexes carrying the SNS/S or the SNN/S donor atom set. Crystal structure of ReO{[(C2H5)2NCH2CH2N(CH2CH2S)2](p-H2N-PhS)} and ReO{[(CH2)4NCH2CH2NCH2CH2S](p-H2N-PhS)}
AUTHOR(S): Papadopoulos, Minas; Tsoukalas, Charalabos; Pirmettis, Ioannis; Nock, Berthold; Maina, Theodosia; Abedin, Zainul; Raptopoulou, Catherine P.; Terzis, Aris; Chiotellis, Efstratios
CORPORATE SOURCE: NCSR 'Demokritos', Institute of Radioisotopes-Radiodiagnostic Products, Aghia Paraskevi, Athens, 15310, Greece
SOURCE: Inorganica Chimica Acta (1999), 285(1), 97-106
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two parallel series of bifunctional mixed ligand oxorhenium and oxotechnetium complexes containing the SNS/S or the SNN/S donor atom set were synthesized

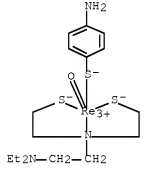
and characterized. The amine bifunctional anchor is positioned on the common monothiolate p-H2N-Ph-SH coligand, which by reacting in equimolar amts. with a tridentate aminethiolate ligand LH2 [LH2 = EtN(CH2CH2SH)2, Et2NCH2CH2N(CH2CH2SH)2, (CH2)4NCH2CH2NHCH2CH2SH and Et2NCH2CH2NHCH2CH2SH] and the corresponding oxometal precursor, gives these series. Two representative members ReO{[Et2NCH2CH2N(CH2CH2S)2](p-H2N-PhS)} and ReO{[(CH2)4NCH2CH2NCH2CH2S](p-H2N-PhS)} are further characterized by crystallog. anal. The SNS/S analogs adopt a distorted trigonal bipyramidal geometry, while the SNN/S ones prefer a distorted square pyramidal geometry around the metal. Extrapolation of structure at tracer level is investigated by chromatog. methods and is established only for the SNS/S, but not for the SNN/S compds. Thus, by this initial evaluation, the applicability of the bifunctional SNS/S (but not the SNN/S) system for tagging biomols. with 99mTc is demonstrated.

IT 178476-48-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure)

RN 178476-48-7 HCAPLUS

CN Rhenium, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

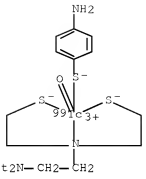


IT 221100-24-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of technetium-99g and -99m oxo aminobenzenethiolato mercaptoethylaminato complexes)

RN 221100-24-9 HCAPLUS

CN Technetium-99Tc, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 24 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:778829 HCAPLUS Full-text
DOCUMENT NUMBER: 130:89625
TITLE: A mixed-ligand P,S,N-cis-dioxorhenium(V) complex by ligand exchange reactions on trans-monooxo-trichlorobis(triphenylphosphine)rhenium(V): formation and structural studies
AUTHOR(S): Friebe, Matthias; Jankowsky, Ruediger; Spies, Hartmut; Seichter, Wilhelm; Papadopoulos, Minas; Chiotellis, Efstratios; Johannsen, Bernd
CORPORATE SOURCE: Forschungszentrum Rossendorf, Institut fur Bioanorganische und Radiopharmazeutische Chemie, Dresden, 01314, Germany
SOURCE: Polyhedron (1998), 17(21), 3711-3720
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

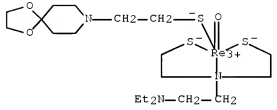
AB In efforts to synthesize Re(V) complexes for potential use in nuclear medicine, tridentate dithiolate ligands were combined with (dialkylamino)ethylenethiols [HS-(CH2)2-NR'2] (R' = alkyl, alkoxy) to form amine-group-bearing mixed-ligand complexes [ReO(SNS)(S)]. Reaction of HSCH2CH2N(CH2CH2NEt2)CH2CH2SH (N,N-bis(2-mercaptoethyl)-N',N'-diethylethylenediamine, 2), as a tris-chelating ligand and 1,4-dioxa-8-azaspiro-N-2-mercaptoethylene-[4,5]-decane (3), with the neutral Re(V) complex [ReOCl3(PPh3)2] (1) yields, in addition to the expected square-pyramidal "3+1" compound (1,4-dioxa-8-azaspiro-N-2-thiolatoethylene- [4,5]-decane){N,N-bis(2-mercaptoethyl)(N',N'- diethylethylenediamine)}oxorhenium(V) (4), the new five-coordinated complex [1,4-dioxa-8-azaspiro-N-2-mercaptoethylene-[4,5]-decane(triphenylphosphine)dioxorhenium(V)] (5). Being the only product in the absence of the tridentate component, 5 has a trigonal-bipyramidal structure, where the coordination sphere is formed by two oxo groups in an uncommon cis-arrangement, S and N from the aminothiolate and by the P atom from the phosphine group originating from the precursor mol. The structure was verified by mass, 1H NMR, IR spectroscopy as well as by XRD. Extended x-ray absorption spectroscopy (EXAFS) was applied to both the precursor and the resulting compound 5 to compare the complex structures in the solid and the

solid states. Expts. with 18O-labeled H2O added to the reaction mixture led to 18O in the dioxo core, showing that H2O is the origin of the addnl. oxo group.

IT 218788-15-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 218788-15-9 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1,4-dioxa-8-azaspiro[4.5]decane-8-ethanethiolato-κS8)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 25 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:655433 HCAPLUS Full-text

DOCUMENT NUMBER: 130:32211

TITLE: Interaction of [ReO(SNS)(S)] and [99mTcO(SNS)(S)] mixed ligand complexes with glutathione: isolation and characterization of the product

AUTHOR(S): Pelecanou, M.; Pirmettis, I. C.; Nock, B. A.; Papadopoulos, M.; Chiotellis, E.; Stassinopoulou, C. I.

CORPORATE SOURCE: Inst. Biol., NCSR 'Demokritos', Athens, 153 10, Greece

SOURCE: Inorganica Chimica Acta (1998), 281(2), 148-152
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

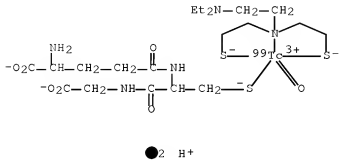
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Interaction of [ReO(Et2NCH2CH2N(CH2CH2S)2)(4-CH3OC6H4S)] (1) with glutathione (GSH) in DMSO-d6 gave [ReO(Et2NCH2CH2N(CH2CH2S)2)(GS)] (2) in which glutathione has replaced the coligand 4-methoxythiophenol. Identification of 2 was achieved by MS, NMR, UV-visible, and IR spectroscopies. The interaction of glutathione with [99mTcO(Et2NCH2CH2N(CH2CH2S)2)(4-CH3OC6H4S)] (3), which is analogous to 1, was also studied at tracer level by HPLC and [99mTcO(Et2NCH2CH2N(CH2CH2S)2)(GS)] is also formed. Complex 3 is a representative of the [99mTcO(SNS)(S)] class of potential brain imaging agents that show high brain uptake and retention in animals tested. The replacement of the coligand 4-methoxythiophenol by glutathione transforms the originally lipophilic complex to hydrophilic; this is being studied further as one of the possible pathways in the retention mechanism of this type of complex.

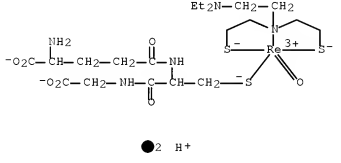
IT 216297-13-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrophilicity)

RN 216297-19-7 HCAPLUS
CN Technetate(2-)-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][L-γ-glutamyl-L-cysteinyl-κS-glycinato(3-)]oxo-, dihydrogen, (SP-5-34)- (9CI) (CA INDEX NAME)



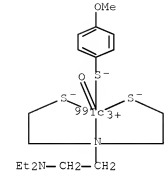
2 H+

IT 216297-15-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 216297-15-3 HCAPLUS
CN Rhenate(2-), [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][L-γ-glutamyl-L-cysteinyl-κS-glycinato(3-)]oxo-, dihydrogen, (SP-5-34)- (9CI) (CA INDEX NAME)

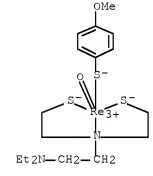


2 H+

IT 158846-32-3 182824-20-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with glutathione)
RN 158846-32-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 182824-20-0 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT:	35	THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (36 CITINGS)
REFERENCE COUNT:	22	THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 26 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

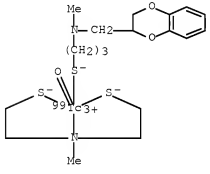
ACCESSION NUMBER:	1998:438102 HCAPLUS Full-text
DOCUMENT NUMBER:	129:257025
ORIGINAL REFERENCE NO.:	129:52282h,52283a
TITLE:	Stability versus reactivity of "3+1" mixed-ligand technetium-99m complexes in vitro and in vivo
AUTHOR(S):	Syhre, R.; Seifert, S.; Spies, H.; Gupta, A.; Johannsen, B.
CORPORATE SOURCE:	Forschungszentrum Rossendorf, Institut fur Bioanorganische und Radiopharmazeutische Chemie, PF 510 119, Dresden, D-01314, Germany
SOURCE:	European Journal of Nuclear Medicine (1998), 25(7), 793-796 CODEN: EJNMD9; ISSN: 0340-6997
PUBLISHER:	Springer-Verlag
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Technetium-99m "3+1" mixed-ligand complexes as relevant to the development of a third generation of 99mTc radiopharmaceuticals were investigated in vivo and in vitro in the blood of rats. Surprisingly, in whole blood the complexes, which proved to be stable in saline, PBS of pH 7.4 and in plasma, were converted into two radioactive, more hydrophilic metabolites. Small structural differences in the complex mol. have a profound influence on the rate of metabolism of the complexes. To obtain an understanding of this unexpected reactivity, transchelation reactions with glutathione (GSH) were hypothesized and this hypothesis substantiated by challenge expts. carried out with a series of 99mTc and analogous rhenium complexes and GSH. In vitro studies in human plasma, whole blood and erythrocytes also revealed conversion of the complexes, though, at a much slower rate. Structural parameters influencing the stability of the complexes and consequences for the radiopharmaceutical design are discussed.

IT 202717-96-2 207567-05-3
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(stability vs. reactivity of "3+1" mixed-ligand technetium-99m complexes in vitro and in vivo)

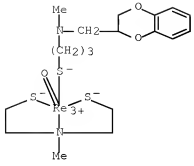
RN 202717-96-2 HCAPLUS

CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



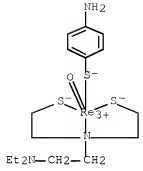
RN 207567-05-3 HCAPLUS

CN Rhenium, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

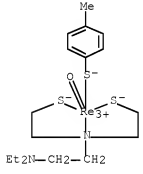


OS.CITING REF COUNT: 59 THERE ARE 59 CAPLUS RECORDS THAT CITE THIS RECORD (59 CITINGS)
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

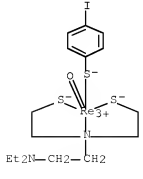
L13 ANSWER 27 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:391750 HCAPLUS Full-text
DOCUMENT NUMBER: 129:130441
ORIGINAL REFERENCE NO.: 129:26521a
TITLE: Synthesis, structure, lipophilicity and protonation behavior of mixed ligand rhenium chelates functionalized by amine groups
AUTHOR(S): Papadopoulos, M.; Pirmettis, I.; Raptopoulou, C.; Chiotellis, E.; Friebe, M.; Berger, R.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Institutes of Radioisotopes-Radiodiagnostic Products and Materials Science, NCSR "Demokritos", Athens, 15310, Greece
SOURCE: Applied Radiation and Isotopes (1998), 49(8), 961-966
CODEN: ARISEF; ISSN: 0969-8043
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Systematically altered neutral oxorhenium complexes ReO[Et2NCH2CH2N(CH2CH2S)2][p-X-C6H4-S] where X = NH2 (1), OMe (2), Me (3), t-Bu (4), H (5), Cl (6), Br (7), I (8), NO2 (9) was prepared by simultaneous action of Et2NCH2CH2N(CH2CH2SH)2 and p-XC6H4SH on [ReOCl3(PPh3)2]. The mol. structure of complex 6 (X = Cl) was determined by x-ray crystallog., revealing a trigonal bipyramidal geometry. PHPLC/pH profiles and pKa values were determined by HPLC.
IT 178476-48-7 178476-50-1 178476-55-6
182824-20-0
RL: PRP (Properties)
(lipophilicity and protonation behavior)
RN 178476-48-7 HCAPLUS
CN Rhenium, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-50-1 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

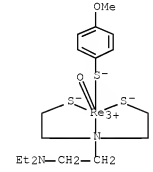


RN 178476-55-6 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-iodobenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

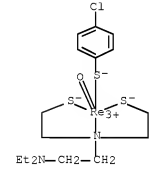


RN 182824-20-0 HCAPLUS

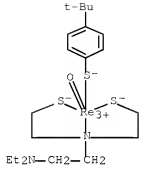
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



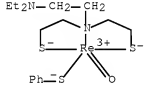
IT 178476-53-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, lipophilicity and protonation behavior)
RN 178476-53-4 HCAPLUS
CN Rhenium, (4-chlorobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



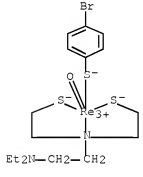
IT 178476-51-2P 178476-52-3P 178476-54-5P
178476-56-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, lipophilicity and protonation behavior)
RN 178476-51-2 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



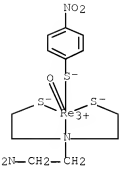
RN 178476-52-3 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-54-5 HCAPLUS
CN Rhenium, (4-bromobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-56-7 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-nitrobenzenethiolato-κS)oxo-, (TB-5-14)- (CA INDEX NAME)



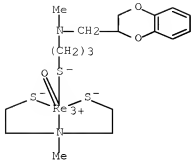
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 28 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190673 HCAPLUS Full-text
DOCUMENT NUMBER: 129:14840
ORIGINAL REFERENCE NO.: 129:3163a,3166a
TITLE: The influence of selected "3+1"oxorhenium(V) complexes on the activity of monoamine oxidase in rat brain homogenate
AUTHOR(S): Matys, S.; Brust, P.; Scheunemann, M.; Pietzsch, H. J.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 135-138
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB Seven oxorhenium complexes with a protonable N in the mol. were tested for their ability to inhibit the monoamine oxidase (MAO) activity in rat brain homogenate. Considering the both MAO isoforms A and B, tryptamine (MAO A and B) and Ph ethylamine (MAO B) were used as substrates. Inhibition expts. involving pargyline (MAO A and B), clorgyline (MAO A), and (-)deprenyl (MAO B) resulted in IC50 values of 0.41, 0.25, and 0.53 μM, resp. A ratio of 80% MAO A to 20% MAO B was found in the brain preparation Inhibition expts. with the Re complexes gave IC50 values between 10-4 and 10-6 M. A Ph group contained in all the oxorhenium complexes acted as an anchor on the active site of MAO. Thus the para-substitution by F led to a 10-fold increase in affinity towards MAO A and B and shifted the selectivity of the mol. towards MAO B. A carbonyl group related to the Ph moiety decreased the affinity.

IT 207567-05-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
("3+1"oxorhenium(V) complexes effect on monoamine oxidase activity in brain homogenate)

RN 207567-05-3 HCAPLUS
CN Rhenium, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

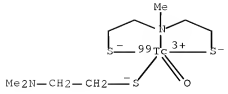


L13 ANSWER 29 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190671 HCAPLUS Full-text
DOCUMENT NUMBER: 128:313494
ORIGINAL REFERENCE NO.: 128:62033a,62036a
TITLE: Are there differences in lipophilicity between the transition metals technetium and rhenium?
AUTHOR(S): Berger, R.; Friebe, M.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 128-131
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

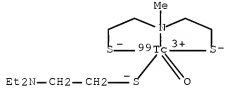
AB PHPLC values (lipophilicity) of neutral complexes MO(SXS)S-(CH2)2-NR2 (M = Tc, Re; NR2 = NMe2, NEt2, NBu2, Pip, Mor; X = S, O, NMe, NEt, NPr, NBu) were measured to verify the influence of M. Reasons of the higher lipophilicity of the Tc compds. are discussed.

IT 178443-28-2 178443-29-3 178443-31-7
190580-27-9 190580-28-0 190580-29-1
190580-32-6 190580-33-7 190580-34-8
190588-01-3 190588-02-4 190588-03-5
190588-06-8 190588-07-9 190588-08-0
190588-11-5 190588-12-6 190588-13-7
206761-53-7 206761-54-8 206761-55-9
206761-58-2 206761-59-3 206761-60-6
RL: PRP (Properties)
(differences in lipophilicity between thioether oxo complexes of Tc and Re)

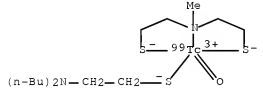
RN 178443-28-2 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



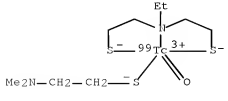
RN 178443-29-3 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 178443-31-7 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

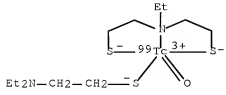


RN 190580-27-9 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

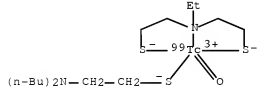


RN 190580-28-0 HCAPLUS

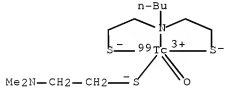
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



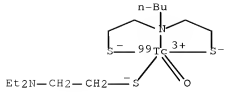
RN 190580-29-1 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



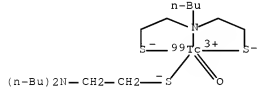
RN 190580-32-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



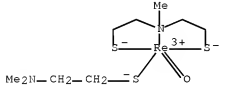
RN 190580-33-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



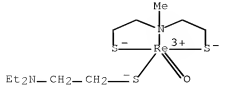
RN 190580-34-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190588-01-3 HCAPLUS
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

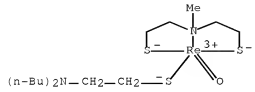


RN 190588-02-4 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



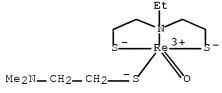
RN 190588-03-5 HCAPLUS

CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



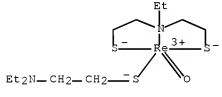
RN 190588-06-8 HCAPLUS

CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



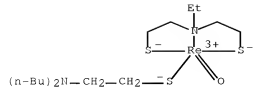
RN 190588-07-9 HCAPLUS

CN Rhenium, [2-(diethylamino)ethanethiolato-κS][2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

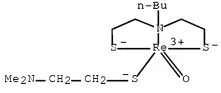


RN 190588-08-0 HCAPLUS

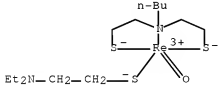
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



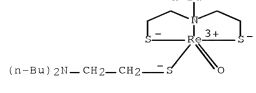
RN 190588-11-5 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-12-6 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

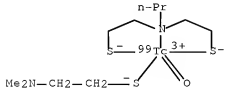


RN 190588-13-7 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



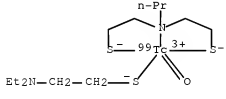
RN 206761-53-7 HCAPLUS

CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



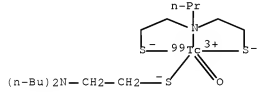
RN 206761-54-8 HCAPLUS

CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)



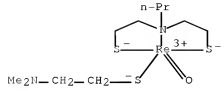
RN 206761-55-9 HCAPLUS

CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)-(9CI) (CA INDEX NAME)

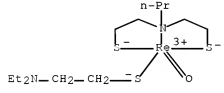


RN 206761-58-2 HCAPLUS

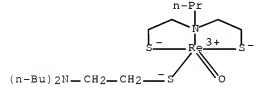
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 206761-59-3 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 206761-60-6 HCAPLUS
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

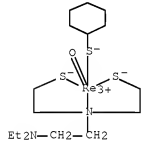
L13 ANSWER 30 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190651 HCAPLUS Full-text
DOCUMENT NUMBER: 128:267786
ORIGINAL REFERENCE NO.: 128:52947a,52950a
TITLE: Rhenium and technetium mixed-ligand chelates functionalized by amine groups. Part 2. Rhenium and technetium complexes with alkyl thiols as monodentate ligands. Preparation, logP/pKa determination, and biodistribution studies
AUTHOR(S): Friebe, M.; Spies, H.; Berger, R.; Johannsen, B.; Papadopoulos, M.; Pirmettis, I.; Maina, T.; Nock, B.; Chiotellis, E.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314,

Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 61-65
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB A series of Tc/Re complexes containing an amine bearing tridentate ligand and coligands with alkyl groups were synthesized, their logP and pKa values were determined, and their distribution patterns were compared with those of complexes with aromatic moieties as coligands. The Re(V) complexes were synthesized by the reaction of trans-monooxotrichlorobis(triphenyl- phosphine) Re(V) with stoichiometric amts. of a mixture of the tridentate and the monodentate ligand in alkaline methanolic solution Yields were 5% in the case of methane thiol to ≈35% in the case of cyclohexane thiol as a monodentate ligand. The "3+1" 99mTc oxotechnetium(V) complexes were prepared by ligand exchange reaction at 99mTc glucoheptonate. All compds. showed a high lipophilicity (P: 310-15,000), the pKa values ranged from 8.13-8.32. Biodistribution studies were carried out on mice. There was no substantial difference between arylic and aliphatic-thiol-substituted complexes concerning their ability to penetrate into the brain. This ability was due to meeting the lipophilicity criteria and a pK that ensured neutrality of a high portion of the complex at pH 7.4.

IT 205578-06-9P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation, crystal and mol. structure, logP/pKa determination, and biodistribution of Re and Tc mixed-ligand chelates functionalized by amine groups and alkyl thiols as monodentate ligands)

RN 205578-06-9 HCAPLUS
CN Rhenium, (cyclohexanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)

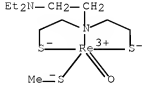


IT 205578-02-5P 205578-03-6P 205578-04-7P
205578-05-8P 205578-07-0P 205578-08-1P
205578-09-2P 205578-10-5P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation, logP/pKa determination, and biodistribution of Re and Tc mixed-ligand
chelates functionalized by amine groups and alkyl thiols as monodentate

ligands)

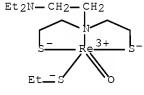
RN 205578-02-5 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](methanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



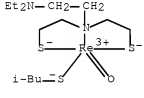
RN 205578-03-6 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](ethanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



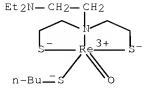
RN 205578-04-7 HCAPLUS

CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](2-methyl-1-propanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

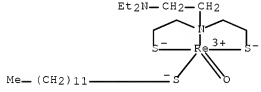


RN 205578-05-8 HCAPLUS

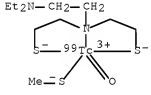
CN Rhenium, (1-butanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



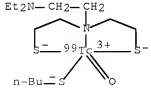
RN 205578-07-0 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1-dodecanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205578-08-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](methanethiolato)oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

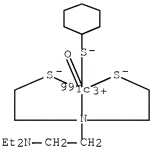


RN 205578-09-2 HCAPLUS
CN Technetium-99Tc, (1-butanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205578-10-5 HCAPLUS
CN Technetium-99Tc, (cyclohexanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA

INDEX NAME)



L13 ANSWER 31 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190650 HCAPLUS Full-text
DOCUMENT NUMBER: 128:267785
ORIGINAL REFERENCE NO.: 128:52947a,52950a
TITLE: Structural modification of the tridentate ligand of n.c.a. "3+1" oxotechnetium(V) mixed-ligand complexes and their effects on the distribution and retention behavior in rats
AUTHOR(S): Syhre, R.; Berger, R.; Brust, P.; Pietzsch, H. J.; Seifert, S.; Scheunemann, M.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 58-60
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

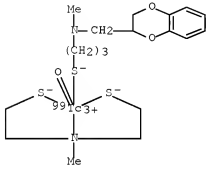
AB The in vivo behavior of various n.c.a. (no carrier added) prepared neutral, lipophilic Tc mixed-ligand complexes are discussed in comparison with the corresponding receptor-affine carrier added complexes. Modification of the 99mTc chelate unit had significant influence on the distribution and retention behavior of the complexes. A considerable amount of all complexes accumulated in the rat kidneys. The liver uptake was lowest for the S-S-S parent compds. compared with the N-alkyl derivs. All complexes penetrated the blood-brain barrier. The brain uptake of the S-S-S parent compound derived complexes correlated to their increasing lipophilicity, and only a slow washout from the brain was observed for these complexes. Independently of the comparable lipophilic parameters, the brain uptake of the N-alkylated complexes was lower and the washout faster than that of the S-S-S parent compds. The accumulation of all investigated complexes was relatively high in the lung after 5 min. Only the modified complexes were rapidly cleared from the lungs. In summary, the presence of the N-alkyl chelate unit accelerated the distribution and retention behavior of the "3+1" oxotechnetium(V) mixed-ligand complexes in rat, but a low brain uptake and no specific accumulation of radioactivity in the receptor-rich brain regions was also found.

IT 202717-96-2 202717-97-3 202717-98-4
205577-78-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structural modification of tridentate ligand of n.c.a. "3+1"

oxotechnetium(V) mixed-ligand complexes and their effects on biodistribution and retention behavior in rat brains and lungs)

RN 202717-96-2 HCAPLUS

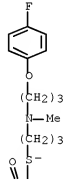
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



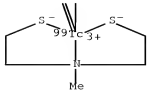
RN 202717-97-3 HCAPLUS

CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

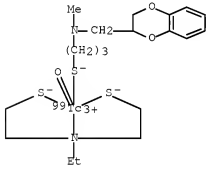
PAGE 1-A



PAGE 2-A

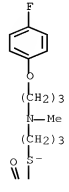


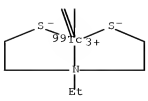
RN 202717-98-4 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205577-78-2 HCAPLUS
CN Technetium-99Tc, [[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)][3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

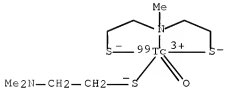
L13 ANSWER 32 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190649 HCAPLUS Full-text
DOCUMENT NUMBER: 128:267784
ORIGINAL REFERENCE NO.: 128:52947a,52950a
TITLE: Structural modifications of carrier added "3+1" oxotechnetium (V) mixed-ligand complexes to improve their blood pool activity in rats
AUTHOR(S): Syhre, R.; Berger, R.; Brust, P.; Friebe, M.; Pietzsch, H. J.; Seifert, S.; Scheunemann, M.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 55-57
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB To improve their blood pool activity, the chelate unit of neutral, lipophilic 99/99mTc "3+1" oxotechnetium(V) mixed ligand complexes containing HS-(CH2)2-S-(CH2)2-SH (X) as tridentate ligands was modified by replacing the X = S by X = O, or X = N-alkyl. The N-alkyl chelates were rapidly cleared from the blood of rats, so that the presence of an N-alkyl group in the tridentate ligand seems to be important for the design of a 99mTc radiopharmaceutical with low background activity in the blood based on the "3+1" concept.

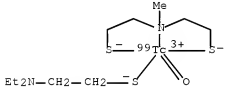
IT 178443-28-2 178443-29-3 190580-27-9
190580-28-0 202717-96-2 202717-97-3
202717-98-4 205577-78-2 205577-84-0
205577-85-1 205577-88-4 205577-89-5
205577-90-8 205577-98-6 205578-00-3
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(blood pool activity and liver uptake affected by structural modifications of carrier added "3+1" oxotechnetium (V) mixed-ligand complexes)

RN 178443-28-2 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-

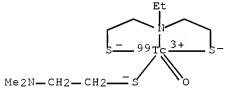
(9CI) (CA INDEX NAME)



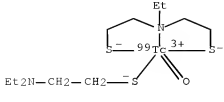
RN 178443-29-3 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



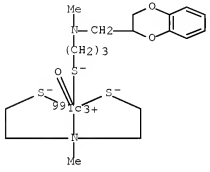
RN 190580-27-9 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



RN 190580-28-0 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)

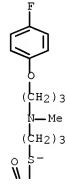


RN 202717-96-2 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

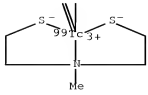


RN 202717-97-3 HCAPLUS
CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

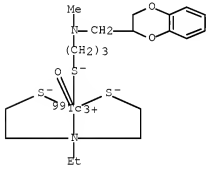
PAGE 1-A



PAGE 2-A

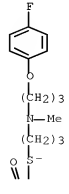


RN 202717-98-4 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

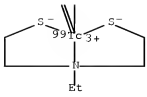


RN 205577-78-2 HCAPLUS
CN Technetium-99Tc, [[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)][3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

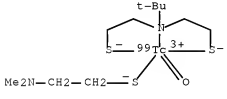
PAGE 1-A



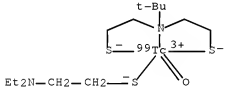
PAGE 2-A



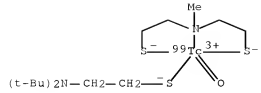
RN 205577-84-0 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



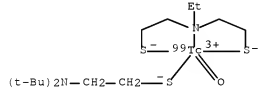
RN 205577-85-1 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



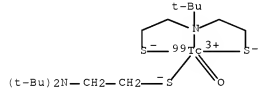
RN 205577-88-4 HCAPLUS
CN Technetium-99Tc, [2-[bis(1,1-dimethylethyl)amino]ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205577-89-5 HCAPLUS
CN Technetium-99Tc, [2-[bis(1,1-dimethylethyl)amino]ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

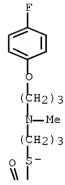


RN 205577-90-8 HCAPLUS
CN Technetium-99Tc, [2-[bis(1,1-dimethylethyl)amino]ethanethiolato-κS][[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

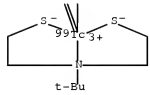


RN 205577-98-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)][3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

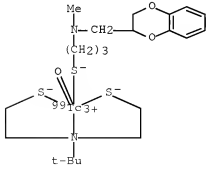
PAGE 1-A



PAGE 2-A



RN 205578-00-3 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-[(1,1-dimethylethyl)imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



L13 ANSWER 33 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:190633 HCAPLUS Full-text
DOCUMENT NUMBER: 128:267782
ORIGINAL REFERENCE NO.: 128:52947a,52950a
TITLE: Serotonin receptor-binding technetium and rhenium complexes. Part 18. Autoradiographical studies of serotonin receptor-binding Tc-99m complexes on post-mortem human brains
AUTHOR(S): Pietzsch, H. J.; Hall, H.; Seifert, S.; Scheunemann, M.; Brust, P.; Spies, H.; Halldin, C.; Johannsen, B.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 14-15
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

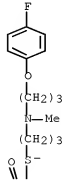
AB Post-mortem human brain autoradiog. studies were performed with 99mTc-oxotechnetium(V) complexes showing substantial in vitro serotonin and dopamine receptor binding in the 2-5 nM range in radiotracer displacement assays. None of the compds. exhibited substantial binding to the sections. The compds. studied possessed Ki-values of 1-2 nM, and this affinity is apparently too low for a 99mTc-labeled tracer.

IT 202717-97-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(autoradiog. studies of serotonin and dopamin receptor-binding Tc-99m complexes on post-mortem human brains)

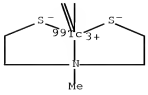
RN 202717-97-3 HCAPLUS

CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

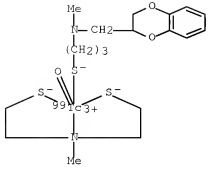


L13 ANSWER 34 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:190632 HCAPLUS Full-text
DOCUMENT NUMBER: 128:289370
ORIGINAL REFERENCE NO.: 128:57141a,57144a
TITLE: Serotonin receptor-binding technetium and rhenium complexes. Part 17. Different routes of n.c.a. preparation of "3+1" 99mTc complexes
AUTHOR(S): Seifert, S.; Pietzsch, H. J.; Scheunemann, M.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Institute Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-200, 10-13
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB A kit-like procedure for preparation of potentially receptor-affine "3+1" 99mTc complexes at the no-carrier-added (n.c.a.) level was examined, involving the reduction of pertechnetate in the presence of the tridentate ligands 3-thiapentane-1,5-dithiol (I) and 3-alkylazapentane-1,5-dithiol (II). Moreover, the role of auxiliary ligands (gluconate, tartrate, citrate, ethylene glycol, propylene glycol, mannitol) was studied for preparing "3+1" 99mTc complexes at n.c.a. level with respect to the development of a reproducible and simple preparation method. Investigations were carried out with the tridentate ligands I and II (N-substituted by a Me, Et, Pr, or pyridinyl group), and 2 of the bulky monothiol ligands used for receptor binding studies, e.g. (2RS)2-[N-(3-mercaptopropyl)-N-methyl-aminomethyl]- 1,4-benzodioxane, and 3-[N-(3-{4-fluorophen-oxy}-propyl)-N-methylamino]- propanethiol. For the formation of "3+1" 99mTc complexes at n.c.a. level with tridentate ligands of the type HS-N(R)-SH, various reaction routes led to high yields of the desired complexes. The direct reduction of pertechnetate eluate in the ligand mixture allowed a kit-like radiopharmaceutical preparation

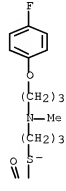
IT 202717-96-2P 202717-97-3P 202717-98-4P
205745-32-0P 205751-20-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 99mTc complexes with tridentate thiol ligands for radiopharmaceutical preparation)

RN 202717-96-2 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

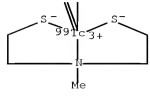


RN 202717-97-3 HCAPLUS
CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A

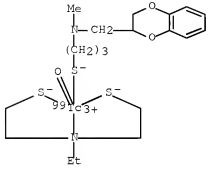


PAGE 2-A

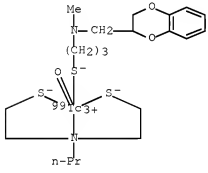


RN 202717-98-4 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-

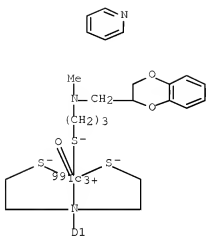
yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205745-32-0 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS]oxo[[2,2'-(propylimino-κN)bis[ethanethiolato-κS]](2-)]-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 205751-20-8 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS]oxo[[2,2'-(pyridinylimino-κN)bis[ethanethiolato-κS]](2-)]- (9CI) (CA INDEX NAME)



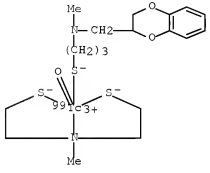
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

L13 ANSWER 35 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:82261 HCAPLUS Full-text
DOCUMENT NUMBER: 128:158892
ORIGINAL REFERENCE NO.: 128:31187a,31190a
TITLE: No carrier added preparations of "3+1" mixed-ligand 99mTc complexes
AUTHOR(S): Seifert, Sepp; Pietzsch, Hans-Juergen; Scheunemann, Matthias; Spies, Hartmut; Syhre, Rosemarie; Johannsen, Bernd
CORPORATE SOURCE: Research Center Rossendorf Inc., Institute of Bioinorganic and Radiopharmaceutical Chemistry, Dresden, 01314, Germany
SOURCE: Applied Radiation and Isotopes (1997), Volume Date 1998, 49(1/2), 5-11
CODEN: ARISEF; ISSN: 0969-8043
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The no carrier added (n.c.a.) preparation of potentially receptor-binding "3+1" mixed-ligand technetium complexes has not so far been successfully accomplished. This article deals with our results in the preparation of n.c.a. Tc complexes with tridentate S-S-S or S-N-S ligands and a series of bulky monothiolato ligands. It was found that Tc(V) gluconate or Tc(V) ethylene glycolate are suitable precursors for the complex formation. In a two-step procedure consisting of a creation of the monothiolato ligand with the precursor and subsequent addition of the tridentate ligand, the desired "3+1" mixed-ligand complexes are formed with yields of up to 90%. Low ligand concns. and pH 9-10 promote the formation of the technetium compds. A comparison of their anal. properties (TLC, HPLC) and biodistribution data of carrier added and no carrier added technetium complexes show the identity of the investigated compds.

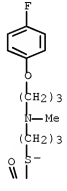
IT 202717-96-2P 202717-97-3P 202717-98-4P
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(no carrier added prepns. of "3+1" mixed-ligand 99mTc complexes)

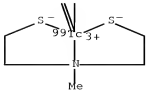
RN 202717-96-2 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



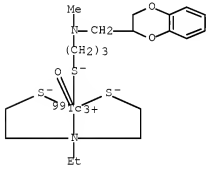
RN 202717-97-3 HCAPLUS
CN Technetium-99Tc, [3-[[3-(4-fluorophenoxy)propyl]methylamino]-1-propanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

PAGE 1-A





RN 202717-98-4 HCAPLUS
CN Technetium-99Tc, [3-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]methylamino]-1-propanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



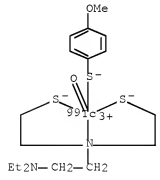
OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS RECORD (30 CITINGS)
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 36 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:528273 HCAPLUS Full-text
DOCUMENT NUMBER: 127:106069
ORIGINAL REFERENCE NO.: 127:20363a,20366a
TITLE: Novel 99mTc Aminobisthiolato/Monothiolato "3 + 1" Mixed Ligand Complexes: Structure-Activity Relationships and Preliminary in Vivo Validation as Brain Blood Flow Imaging Agents
AUTHOR(S): Pirmettis, Ioannis C.; Papadopoulos, Minas S.; Chiotellis, Efstratios
CORPORATE SOURCE: Institute of Radioisotopes-Radiodiagnostic Products, NCSR Demokritos, Athens, Greece
SOURCE: Journal of Medicinal Chemistry (1997), 40(16), 2539-2546
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of neutral, lipophilic 99mTc mixed-ligand complexes of the general formula 99mTcOL1L2, where L1H2 is an N-substituted bis-(2-mercaptoethyl)amine, [X-CH2CH2N(CH2CH2SH)2], [SNS], and L2H is a monodentate thiol (RSH), [S], has

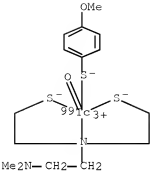
been synthesized and evaluated in rodents for potential use in brain blood flow imaging. The complexes were prepared by ligand exchange reaction using 99mTc(V)O-glucoheptonate as precursor and equimolar quantities of the two ligands. In all cases the syn isomer was formed in a high yield, whereas the anti isomer was not always present. The formation of two isomeric complexes-syn and anti-was expected, since the N-substituent (X-CH2CH2N) can assume syn or anti configuration with respect to the 99mTcO3+ core during complexation. One anti and all syn isomers were isolated by HPLC. Their identity was confirmed by comparative HPLC studies with the analogous 99Tc complexes of established structure. In vivo distribution, in particular brain uptake and retention, greatly depended on the type of either tridentate (L1H2) or monodentate (L2H) ligand. All 99mTc complexes showed significant brain uptake in mice (0.78-4.35% injected dose per organ at 5 min postinjection). This initial uptake remained nearly constant for at least 30 min for most of the complexes. Structure-activity relationships of novel 99mTc(V)O SNS/S complexes in mice are reported and discussed. Selected complexes were further studied in rats. High brain uptake, comparable to that of 99mTc-d,l-HMPAO, and sufficient retention 60 min postinjection were provided with complex 18 [X = (C2H5)2N and R = p-CH3OC6H4CH2].

IT 158846-32-3P 174537-58-7P 174537-60-1P
174537-61-2P 174537-62-3P 174537-63-4P
174537-64-5P 174537-65-6P 174537-66-7P
174537-67-8P 174537-68-9P 174537-69-0P
174537-70-3P 174537-71-4P 174537-74-7P
174537-75-8P 174537-76-9P 174592-02-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and structure activity relations of 99mTc aminobisthiolato/monothiolato mixed ligand complexes and in vivo validation as brain blood flow imaging agents)

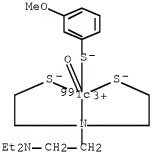
RN 158846-32-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



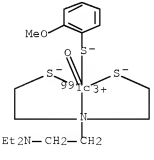
RN 174537-58-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(dimethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 174537-60-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](3-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

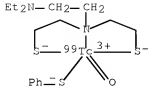


RN 174537-61-2 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](2-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

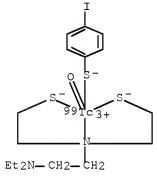


RN 174537-62-3 HCAPLUS
CN Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA

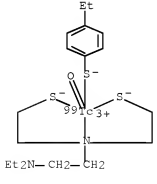
INDEX NAME)



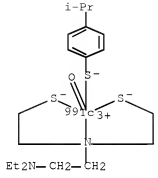
RN 174537-63-4 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-iodobenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



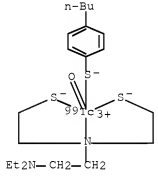
RN 174537-64-5 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-ethylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



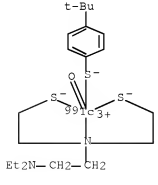
RN 174537-65-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1-methylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



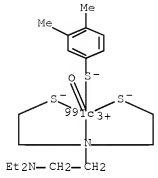
RN 174537-66-7 HCAPLUS
CN Technetium-99Tc, (4-butylbenzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



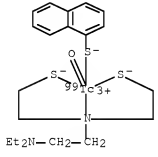
RN 174537-67-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



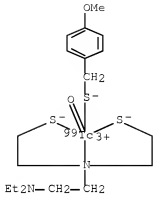
RN 174537-68-9 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](3,4-dimethylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



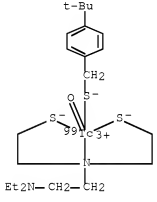
RN 174537-69-0 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1-naphthalenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



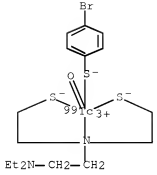
RN 174537-70-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenemethanethiolato-κS)oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



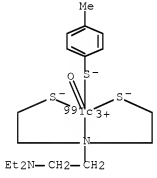
RN 174537-71-4 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenemethanethiolato]oxo-, stereoisomer (9CI) (CA INDEX NAME)



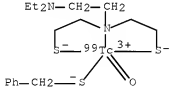
RN 174537-74-7 HCAPLUS
CN Technetium-99Tc, (4-bromobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)



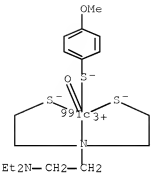
RN 174537-75-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 174537-76-9 HCAPLUS
CN Technetium-99Tc, (benzenemethanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



RN 174592-02-0 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, stereoisomer (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 35 THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (35 CITINGS)
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 37 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:380992 HCAPLUS Full-text
DOCUMENT NUMBER: 126:340548
ORIGINAL REFERENCE NO.: 126:66151a,66154a
TITLE: Dopamine and serotonin transporter ligand tropane-based derivatives, their technetium and rhenium complexes, and preparation thereof, for use as imaging agents for CNS receptors
INVENTOR(S): Kung, Hank F.; Meegalla, Sanath; Kung, Mei-ping; Ploessl, Karl
PATENT ASSIGNEE(S): The Trustees of the University of Pennsylvania, USA; Kung, Hank F.; Meegalla, Sanath; Kung, Mei-Ping; Ploessl, Karl
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9714445	A1	19970424	WO 1996-US16908	19961021 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG				
US 6241963	B1	20010605	US 1996-649782	19960517 <--
CA 2233173	A1	19970424	CA 1996-2233173	19961021 <--
CA 2233173	C	20060404		
AU 9711566	A	19970507	AU 1997-11566	19961021 <--
AU 716235	B2	20000224		
EP 929319	A1	19990721	EP 1996-942721	19961021 <--
EP 929319	B1	20040922		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

JP 11514368	T	19991207	JP 1996-516091		19961021 <--
AT 276770	T	20041015	AT 1996-942721		19961021 <--
PRIORITY APPLN. INFO.:			US 1995-545327	A	19951019 <--
			US 1996-649782	A	19960517 <--
			WO 1996-US16908	W	19961021 <--

OTHER SOURCE(S): MARPAT 126:340548

AB Tropane-based derivs. complexed with either technetium or rhenium that are specific for central nervous system receptors, in particular, dopamine or serotonin receptors, are disclosed. The compds. of the invention have utility, inter alia, as imaging agents for CNS receptors. Methods of using these novel compds. as imaging agents are presented, as are intermediates and methods for making these compds.

IT 190022-00-5P

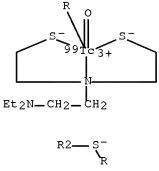
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(dopamine and serotonin transporter ligand tropane-based derivs., technetium and rhenium complexes, preparation, and use as imaging agents for CNS receptors)

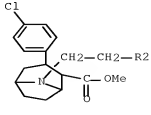
RN 190022-00-5 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][methyl (1R,2S,3S,5S)-3-(4-chlorophenyl)-8-[2-(mercapto-κS)ethyl]-8-azabicyclo[3.2.1]octane-2-carboxylato]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



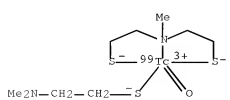
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 38 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:321157 HCAPLUS Full-text
DOCUMENT NUMBER: 127:40549
ORIGINAL REFERENCE NO.: 127:7663a,7666a
TITLE: Lipophilicity and ionization properties of some amine-bearing technetium and rhenium "3+1" mixed ligand chelates of the same ligand structure
AUTHOR(S): Berger, R.; Friebe, M.; Pietzsch, H. J.; Scheunemann, M.; Noll, B.; Fietz, T.; Spies, H.; Johannsen, Bernd
CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-165, 43-47
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB Lipophilicity and ionizability of series of Tc and Re thiolate azapentanedithiolate/thiapentanedithiolate/oxapentanedithiolate complexes, designed for application as brain radiopharmaceuticals, were analyzed by reversed-phase HPLC. From the Tc/Re PHPLC value pairs of the same ligand structure, a higher lipophilicity of the Tc complexes was deduced. The substitution of the central heteroatom in the tridentate ligand increased PHPLC in the order N-Me < N-Et .apprx. S .apprx. O < N-Bu. Prolonging the N-alkyl side chains in the monodentate ligand increased the pKa(c) as well as the PHPLC values. Except from the morpholine derivs., the lipophilicity grew with the number of C atoms in the amine group according to Mor .apprx. NMe2 < NEt2 <Pip < NBu2.

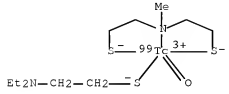
IT 178443-28-2 178443-29-3 178443-31-7
190580-27-9 190580-28-0 190580-32-6
190580-33-7 190588-01-3 190588-02-4
190588-03-5 190588-06-8 190588-07-9
190588-11-5 190588-12-6
RL: PRP (Properties)
(lipophilicity and ionizability studied by reversed-phase HPLC of)

RN 178443-28-2 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

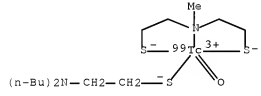


RN 178443-29-3 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-

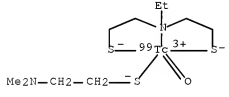
(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



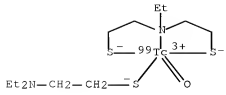
RN 178443-31-7 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-
(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



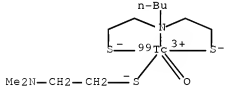
RN 190580-27-9 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-
(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



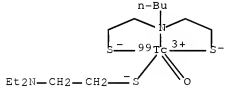
RN 190580-28-0 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-
(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-
(9CI) (CA INDEX NAME)



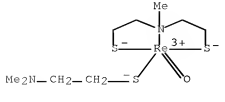
RN 190580-32-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190580-33-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

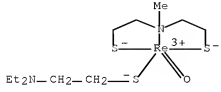


RN 190588-01-3 HCAPLUS
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



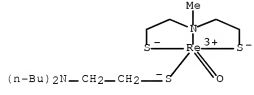
RN 190588-02-4 HCAPLUS

CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



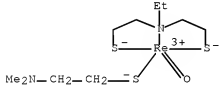
RN 190588-03-5 HCAPLUS

CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



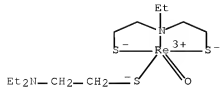
RN 190588-06-8 HCAPLUS

CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

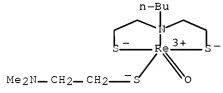


RN 190588-07-9 HCAPLUS

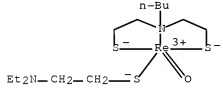
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-11-5 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-12-6 HCAPLUS
CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L13 ANSWER 39 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:321156 HCAPLUS Full-text
DOCUMENT NUMBER: 127:28206
ORIGINAL REFERENCE NO.: 127:5267a,5270a
TITLE: Preparation of amine group-bearing "3+1" mixed-ligand oxotechnetium(V) complexes at the carrier-added level
AUTHOR(S): Friebe, M.; Papadopoulos, M.; Chiotellis, E.; Spies, H.; Berger, R.; Johannsen, Bernd
CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-165, 40-42
CODEN: FRBFEU

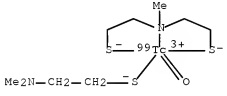
DOCUMENT TYPE: Report
LANGUAGE: English

AB 99'99mTcO(SCH2CH2NR2)(SCH2CH2XCH2CH2S) (X = S, O, NMe, NEt, NBu; NR2 = NME2, NEt2, NBu2, piperidinyl, morpholinyl) were prepared to obtain more information on the structure dependence of the brain uptake of Tc complexes. The compds. were obtained from a 2-step reaction, starting from pertechnetate. At 1st Tc(V) gluconate was prepared, which was subjected to a ligand exchange reaction with a tridentate/monodentate ligand mixture Products were purified by extraction and characterized by thin layer chromatog. and x-ray diffraction anal.

IT 178443-28-2P 178443-29-3P 178443-31-7P
190580-27-9P 190580-28-0P 190580-29-1P
190580-32-6P 190580-33-7P 190580-34-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of stable and metastable)

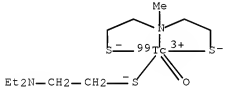
RN 178443-28-2 HCAPLUS

CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



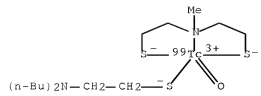
RN 178443-29-3 HCAPLUS

CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

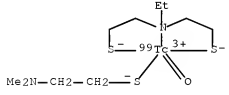


RN 178443-31-7 HCAPLUS

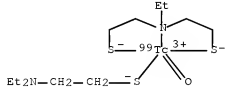
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



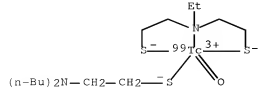
RN 190580-27-9 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190580-28-0 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)

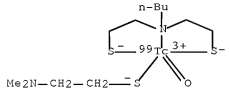


RN 190580-29-1 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



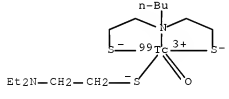
RN 190580-32-6 HCAPLUS

CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



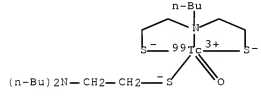
RN 190580-33-7 HCAPLUS

CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 190580-34-8 HCAPLUS

CN Technetium-99Tc, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



L13 ANSWER 40 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:321155 HCAPLUS Full-text

DOCUMENT NUMBER: 127:28205

ORIGINAL REFERENCE NO.: 127:5267a,5270a

TITLE: Synthesis of neutral amine group-bearing "3+1" mixed-ligand oxorhenium(V) complexes

AUTHOR(S): Friebe, M.; Papadopoulus, M.; Chiotellis, S.; Spies, H.; Berger, R.; Johannsen, Bernd

CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany

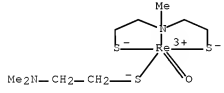
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-165, 35-40
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB ReO(SCH2CH2XCH2CH2S)(SCH2CH2NR2) (X = S, O, NMe, NEt, NBu; NR2 = NMe2, NEt2, NBu2, piperidinyl, morpholinyl) the title compds. were prepared to study the relationship between lipophilicity or basicity and brain uptake of oxometal complexes of Re and Tc. Products were characterized by elemental anal., IR spectroscopy, and HPLC. Structural parameters of 1 selected representative were obtained by EXAFS.

IT 190588-01-3P 190588-02-4P 190588-03-5P
190588-06-8P 190588-07-9P 190588-08-0P
190588-11-5P 190588-12-6P 190588-13-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

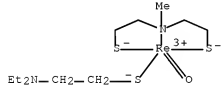
RN 190588-01-3 HCAPLUS

CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



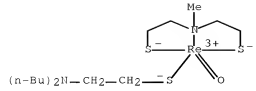
RN 190588-02-4 HCAPLUS

CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

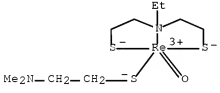


RN 190588-03-5 HCAPLUS

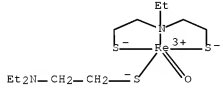
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



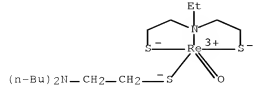
RN 190588-06-8 HCAPLUS
CN Rhenium, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-07-9 HCAPLUS
CN Rhenium, [2-(diethylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)

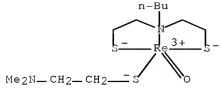


RN 190588-08-0 HCAPLUS
CN Rhenium, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



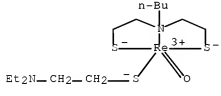
RN 190588-11-5 HCAPLUS

CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dimethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



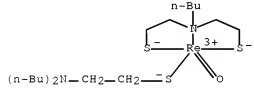
RN 190588-12-6 HCAPLUS

CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(diethylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 190588-13-7 HCAPLUS

CN Rhenium, [[2,2'-(butylimino-κN)bis[ethanethiolato-κS]](2-)][2-(dibutylamino)ethanethiolato-κS]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



L13 ANSWER 41 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:321154 HCAPLUS Full-text

DOCUMENT NUMBER: 127:59824

ORIGINAL REFERENCE NO.: 127:11255a,11258a

TITLE: Serotonin receptor-binding technetium and rhenium complexes. Part 15. Synthesis and characterization of oxorhenium(V) complexes with N-functionalized tridentate SNS ligands

AUTHOR(S): Pietzsch, H. J.; Scheunemann, M.; Berger, R.; Brust, P.; Spies, H.; Johannsen, Bernd

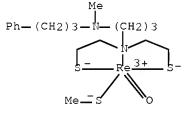
CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry,

Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-165, 32-35
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

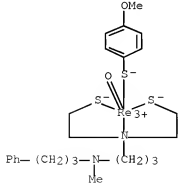
AB Oxorhenium(V) complexes were prepared by ligand exchange reaction of [ReOCl3(PPh3)2] with equimol. amts. of (HSCH2CH2)2N(CH2)nR (n = 3, R = NMeCH2CH2CH2Ph, 4-(phenylmethyl)piperidinyl; n = 2, R = NMeCH2CH2CH2OPh) and 4-MeOC6H4SH or MeSNa. PK values and partition and distribution coeffs. of the complexes are reported.

IT 178443-47-5P 178443-48-6P 191022-08-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, acidity, and partition of)

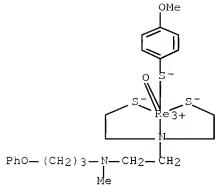
RN 178443-47-5 HCAPLUS
CN Rhenium, (methanethiolato)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 178443-48-6 HCAPLUS
CN Rhenium, (4-methoxybenzenethiolato-κS)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



RN 191022-08-9 HCAPLUS
CN Rhenium, (4-methoxybenzenethiolato-κS)[[2,2'-[[2-[methyl(3-phenoxypropyl)amino]ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



L13 ANSWER 42 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:321152 HCAPLUS Full-text
DOCUMENT NUMBER: 127:106057
ORIGINAL REFERENCE NO.: 127:20363a,20366a
TITLE: Serotonin receptor-binding technetium and rhenium complexes. Part 13. No carrier added preparations of "3+1" 99mTc complexes
AUTHOR(S): Seifert, S.; Pietzsch, H. J.; Scheunemann, M.; Spies, H.; Syhre, R.; Johannsen, Bernd
CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997), FZR-165, 16-22
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

AB Reaction conditions were studied allowing reliable and reproducible preparation of "3+1" Tc complexes at no carrier added (n.c.a.) level with yields and stabilities sufficient for animal studies. Complexation reactions were studied at n.c.a. level with the tridentate ligand L1 = 3-thiapentane-1,5-dithiol or with 3-ethylazapentane-1,5-dithiol and a monodentate thiols L2, e.g. small ligands such as ethanethiol, 2-propanethiol, or larger monothiols like: (2RS) 2-[N-(3-mercaptopropyl)-N-methyl-aminomethyl]-1,4-benzodioxane, 3-[N-(3-{4-fluorophenoxy)-propyl)-N-methylamino]propanethiol, 3-[N-(3-phenoxypropyl)-N-methylamino]propanethiol, 2-[N-(3-phenoxypropyl)-N-methylamino]ethanethiol, (2RS) 2-mercaptomethyl-4-(3-phenylpropyl)morpholine, 3-[2-(N-3-phenylpropyl-N-2-mercaptoethyl)-aminoethyl]-2,4-(1H,3H)-quinazolindione. The complexation reaction proceeded with better yields when an excess of the monodentate ligand L2 was added at 1st. Subsequently L1 was added and the "3+1" complex was formed in a slow reaction. The reaction was accelerated by careful heating at 40° for yields of 80-90%. The best results were obtained with 0.5-0.2 mg of the monothiolato ligand and 0.05-0.02 mg of the tridentate ligand. The optimized prepns. were stable for 2 h at room temperature If the ligand excess was separated the complex solns. were stable for more than 8 h. The monothiols used for complexation changed with time. The best yields were obtained by adding 100 µl 0.1 n NaOH to the 99mTc gluconate solution (pH = 11) and complexation with 0.3-0.5 mg oxalate of the monothiolato ligand and 0.05 mg of the tridentate HS-S-SH ligand. Heating at

40° (60 min) resulted >70% of the complexes. The preparation of 99mTc complexes with thiols like ethanethiol or 2-propanethiol needed other conditions. Tc gluconate reacted immediately with both thiols to the intermediate complex. The optimum temperature for formation of "3+1" complexes was 60°. A diminished monothiol ligand concentration of 0.2 mg and a content of 0.08-0.1 mg per vial of the S-S-S lead to shorter reaction times of 1-2 h and higher yields of 80-90%. The stability of these complexes was higher than that of complexes with bulky ligands. Organ distribution studies performed on rats confirmed the identity of the prepns.

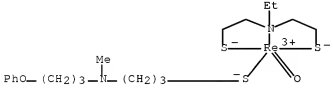
IT 192315-81-4P

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(serotonin receptor-binding no carrier added prepns. of "3+1" 99mTc complexes)

RN 192315-81-4 HCAPLUS

CN Rhenium, [[2,2'-(ethylimino-κN)bis[ethanethiolato-κS]](2-)][3-[methyl(3-phenoxypropyl)amino]-1-propanethiolato-κS]oxo-, (SP-5-43)-(9CI) (CA INDEX NAME)



L13 ANSWER 43 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:98749 HCAPLUS Full-text

DOCUMENT NUMBER: 126:183184

ORIGINAL REFERENCE NO.: 126:35309a

TITLE: Effect of the method of 99mTc labeling of liposomes on their biological behavior

AUTHOR(S): Sabba-Dimopoulou, Ch.; Pirmettis, I.; Archimandriti, M.; Papadopoulos, M.; Chiotellis, E.

CORPORATE SOURCE: Inst. Radioisot. Radiodiagnostic Prod., EKEFE Demokritos, Greece

SOURCE: Chemika Chronika, Genike Ekdose (1996), 58(12), 661-664
CODEN: CCGEAC; ISSN: 0366-5526

PUBLISHER: Enosis Ellenon Chemikon

DOCUMENT TYPE: Journal; General Review

LANGUAGE: Greek

AB A review with 40 refs., including new data on the organ distribution of technetium-99m-labeled liposomes vs. the free technetium-99m-labeled compds. (99mTc-pertechnetate, 99mTcO2, 99mTc-tartrate, 99mTc-SnCl2, and 99mTc-TBTP).

IT 174537-67-8

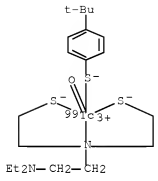
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(effect of the method of 99mTc labeling of liposomes on their biodistribution)

RN 174537-67-8 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-

κN]bis[ethanethiolato-κS]](2-)][4-(1,1-
dimethylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



L13 ANSWER 44 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:694343 HCAPLUS Full-text
DOCUMENT NUMBER: 125:322341
ORIGINAL REFERENCE NO.: 125:60259a,60262a
TITLE: 99Tc-labeled serotonin receptor-binding substances
INVENTOR(S): Johannsen, Bernd; Pietzsch, Hans-Juergen; Scheunemann, Matthias; Spies, Harmut; Brust, Peter
PATENT ASSIGNEE(S): Mallinckrodt Medical, Inc., USA
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9630054	A1	19961003	WO 1996-US4239	19960327 <--
W: CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			EP 1995-200771 A	19950328 <--

OTHER SOURCE(S): MARPAT 125:322341

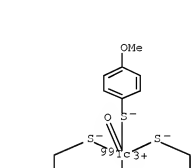
AB A zero-charged 99mTc-labeled substance having serotonin receptor-binding activity, for use as a radiopharmaceutical and for medical imaging of tissues containing serotonin receptors, has the formula LABE [L = chelating moiety comprising a tridentate/monodentate chelating combination; A = 2-8-membered hydrocarbon biradical optionally containing 1 or 2 O and/or S atoms; B = NR, (substituted) piperidine-, piperazine-, morpholine-, or pyrrolidine-derived biradical; R = H, C1-4 alkyl; E = aryl, heteroaryl; or BE = (substituted) 2,4-dihydroquinazolyl] labeled with 99mTc in the form of oxotechnetium(V) attached to the chelating moiety. Thus, N-(2-mercaptoethyl)-N-methyl-3-phenylpropylamine (I) was prepared by condensation of N-methylaminoethanol with 3-phenylpropyl chloride, followed by reaction with HCl, SOCl2, and thiourea. A tridentate/monodentate complex was prepared by reaction of 99mTc gluconate with equimolar amts. of I and S-(2-mercaptoethyl)ethane-1,2-thiol. This complex bound to serotoninergic 2A receptors in rat brain cortex homogenates with a binding constant similar to that for ketanserin.

IT 183312-26-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(technetium-labeled serotonin receptor-binding substances)

RN 183312-26-7 HCAPLUS

CN Technetium-99Tc, (4-methoxybenzenethiolato-S)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino]bis[ethanethiolato]](2-)]oxo-, (SP-5-34)-(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 45 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:678784 HCAPLUS Full-text

DOCUMENT NUMBER: 125:315098

ORIGINAL REFERENCE NO.: 125:58659a

TITLE: Syn-Anti Isomerism in a Mixed-Ligand Oxorhenium Complex, ReO[SN(R)S][S]

AUTHOR(S): Papadopoulos, M. S.; Pirmettis, I. C.; Pelecanou, M.; Raptopoulou, C. P.; Terzis, A.; Stassinopoulou, C. I.; Chiotellis, E.

CORPORATE SOURCE: Institutes of Radioisotopes-Radiodiagnostic Products Biology, NCSR Demokritos, Athens, Greece

SOURCE: Inorganic Chemistry (1996), 35(25), 7377-7383
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

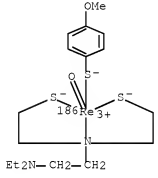
DOCUMENT TYPE: Journal

LANGUAGE: English

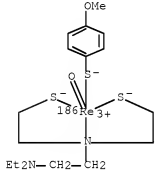
AB The simultaneous action of the tridentate ligand Et2NCH2CH2N(CH2CH2SH)2 and the monodentate coligand HSC6H4OCH3 on a suitable ReO3+ precursor results in a mixture of syn- and anti-oxorhenium complexes, ReO[Et2NCH2CH2N(CH2CH2S)2][SC6H4OCH3], in a ratio of 25/1. The complexes were prepared by a ligand exchange reaction using ReO(eg)2 (eg = ethylene glycol), ReOCl3(PPh3)2, or Re(V)-citrate as precursor. Both complexes were characterized by elemental anal., FTIR, UV-visible, x-ray crystallog., and NMR spectroscopy. The syn isomer crystallizes in the monoclinic space group P21/n, a 14.109(4), b 7.518(2), c 20.900(5) Å, β 103.07(1)°, Z = 4. The anti isomer crystallizes in space group P21/n, a 9.3850(7), b 27.979(2), c 8.3648(6) Å, β 99.86(1)°, Z =

4. Complete NMR studies show that the orientation of the N substituent chain with respect to the Re:O core greatly influences the observed chemical shifts. Complexes were also prepared at the tracer (186Re) level by using 186Re-citrate as precursor. Corroboration of the structure at tracer level was achieved by comparative HPLC studies.

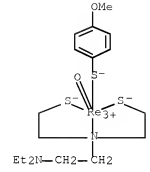
IT 182676-05-7P 182824-21-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and solid and solution mol. structure of)
RN 182676-05-7 HCAPLUS
CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino]bis[ethanethiolato]](2-)](4-methoxybenzenethiolato-S)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



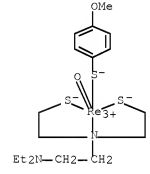
RN 182824-21-1 HCAPLUS
CN Rhenium-186Re, [[2,2'-[[2-(diethylamino)ethyl]imino]bis[ethanethiolato]](2-)](4-methoxybenzenethiolato-S)oxo-, stereoisomer (9CI) (CA INDEX NAME)



IT 178476-49-8P 182824-20-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal and solution structure, and fluxionality of)
RN 178476-49-8 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino]bis[ethanethiolato]](2-)](4-methoxybenzenethiolato-S)oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



RN 182824-20-0 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 56 THERE ARE 56 CAPLUS RECORDS THAT CITE THIS RECORD (57 CITINGS)

L13 ANSWER 46 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:393877 HCAPLUS Full-text
DOCUMENT NUMBER: 125:52471
ORIGINAL REFERENCE NO.: 125:9984h,9985a
TITLE: Tc-99m-Labeled Tropanes as Dopamine Transporter Imaging Agents
AUTHOR(S): Meegalla, Sanath; Ploessl, Karl; Kung, Mei-Ping; Chumpradit, Sumalee; Stevenson, D. Andrew; Frederick, Dana; Kung, Hank F.
CORPORATE SOURCE: Departments of Radiology and Pharmacology, University of Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Bioconjugate Chemistry (1996), 7(4), 421-429
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The development of novel Tc-99m-labeled tropane derivs. as dopamine transporter imaging agents is reported. A series of neutral and lipophilic conjugated complexes, containing N-(alkylthiolato)tropane,

aminobis(ethylthiolato), and a [99mTc]TcO3+ center core, was prepared and evaluated as central nervous system (CNS) dopamine transporter imaging agents in rats. One of the compds., [99mTc]technetium, [methyl 3-(4-chlorophenyl)-8-(2-mercaptoethyl)-8-azabicyclo[3.2.1]octane-2- carboxylato-S][[2,2'-(methylimino)bis[ethanethiolato]](2-)-N,S,S']oxo (25), displayed low initial uptake in rat brain (0.1% at 2 min post i.v. injection); the striatal/cerebellar (ST/CB) ratio reached 3.50 at 60 min after an i.v. injection. The specific uptake can be blocked by pretreating rats with a competing dopamine transporter binding agent, β-CIT (RTI-55, N-methyl-2β-carbomethoxy-3β-(4- iodophenyl)tropane; i.v., 1 mg/kg), which reduced the regional brain uptake ratio (ST/CB) to 1.0. In contrast, the specific uptake in striatum was not affected by pretreating rats with a noncompeting ligand, haldol (i.v., 1 mg/kg). In vitro autoradiog. of rat brain sections exhibited elevated labeling in striatum, major islands of Calleja, and olfactory tubercle regions, where dopamine neurons are known to be concentrated This series of compds. is the first example of technetium-99m labeled CNS receptor-specific imaging agents and may provide a convenient source of short-lived imaging agents for routine diagnosis of CNS abnormality in conjunction with single photon emission computed tomog.

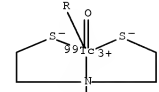
IT 177351-79-0P

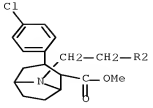
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(metastable; 99mTc-labeled tropanes as brain dopamine transporter SPECT agents)

RN 177351-79-0 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][methyl 3-(4-chlorophenyl)-8-[2-(mercapto-κS)ethyl]-8-azabicyclo[3.2.1]octane-2-carboxylato]oxo-, [SP-5-31-(exo,exo)]- (9CI) (CA INDEX NAME)

PAGE 1-A





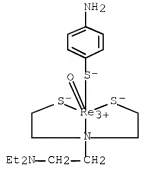
OS.CITING REF COUNT: 46 THERE ARE 46 CAPLUS RECORDS THAT CITE THIS RECORD (47 CITINGS)

L13 ANSWER 47 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:295744 HCAPLUS Full-text
DOCUMENT NUMBER: 125:80669
ORIGINAL REFERENCE NO.: 125:15170h,15171a
TITLE: Rhenium and technetium mixed-ligand chelates functionalized by amine groups. Part 1. Rhenium complexes with p-substituted benzenethiols as monodentate ligands
AUTHOR(S): Papadopoulos, M.; Chiotellis, S.; Spies, H.; Friebe, M.; Berger, R.; Johannsen, B.
CORPORATE SOURCE: Inst. Radioisotopes Radiodiagnostic Products, Natl. Cent. Sci. Res. "Demokritos", Athens, Greece
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1996), FZR-122, 80-82
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

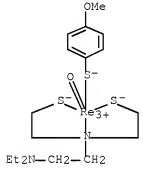
AB The preparation and characterization of rhenium complexes used as radiotracers for CNS, where the tridentate ligand SNS contains a pendant diethylaminoethyl group and the monodentate benzenethiol is varied in the p-position by substituents, is described. Lipophilicity data log P and log D and pK values are given. Apart from compound log P = 1.64, the values of log P are in the range of 3.0-4.6. The corresponding log D values (at pH 7.4) are 1 logarithmic unit lower. The pK values, varying in a very limited region of 8.3-8.0.

IT 178476-48-7P 178476-49-8P 178476-50-1P
178476-51-2P 178476-52-3P 178476-53-4P
178476-54-5P 178476-55-6P 178476-56-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(rhenium chelate complexes containing p-substituted monodentate benzothiazoles preparation and characterization)

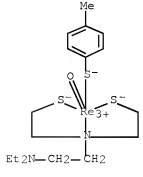
RN 178476-48-7 HCAPLUS
CN Rhenium, (4-aminobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-49-8 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino]bis[ethanethiolato]](2-)](4-methoxybenzenethiolato-S)oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)

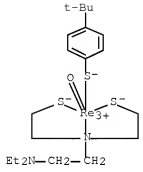


RN 178476-50-1 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

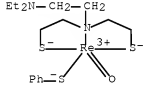


RN 178476-51-2 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-

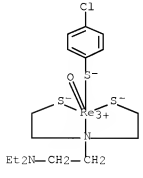
κS]](2-)][4-(1,1-dimethylethyl)benzenethiolato]oxo-, (TB-5-14)-
(9CI) (CA INDEX NAME)



RN 178476-52-3 HCAPLUS
CN Rhenium, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA
INDEX NAME)

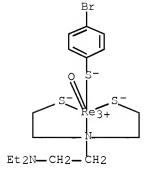


RN 178476-53-4 HCAPLUS
CN Rhenium, (4-chlorobenzenethiolato-κS)[[2,2'-[[2-
(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-,
(TB-5-14)- (9CI) (CA INDEX NAME)

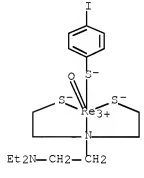


RN 178476-54-5 HCAPLUS
CN Rhenium, (4-bromobenzenethiolato-κS)[[2,2'-[[2-

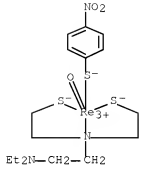
(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-,
(TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-55-6 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-iodobenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 178476-56-7 HCAPLUS
CN Rhenium, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-nitrobenzenethiolato-κS)oxo-, (TB-5-14)- (CA INDEX NAME)

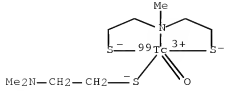


L13 ANSWER 48 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:295743 HCAPLUS Full-text
DOCUMENT NUMBER: 125:80555
ORIGINAL REFERENCE NO.: 125:15143a,15146a
TITLE: pKa value determinations by HPLC of some Tc and Re complexes containing an ionizable group
AUTHOR(S): Berger, R.; Scheunemann, M.; Pietzsch, H. J.; Noll, B.; Noll, S.; Hoepping, A.; Glaser, M.; Fietz, T.; Spies, H.; Johannsen, B.
CORPORATE SOURCE: Inst. Bioinorg. Radiopharm. Chem., Res. Cent. Rossendorf Inc., Dresden, D-01314, Germany
SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1996), FZR-122, 73-79
CODEN: FRBFEU
DOCUMENT TYPE: Report
LANGUAGE: English

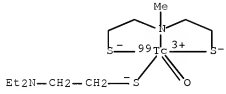
AB Neutral Tc and Re chelate complexes bearing a tertiary amine group of a weak basic character and similar complexes with a functional group with acid properties in the side chain were investigated. The ionization constant (pKa) was determined by HPLC with MeCN as solvent as well as partition coeffs. (P). Lengthening of the N-alkyl side chains increase both the pK and P values and Tc and Re complexes prepared from the same ligands have identical pK values. The P values of the unionized chelates show a similar relation as above described.

IT 178443-28-2 178443-29-3 178443-30-6
178443-31-7 178443-47-5 178443-48-6
RL: PRP (Properties)
(pKa determination of Tc and Re complexes containing an ionizable group by HPLC)

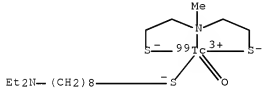
RN 178443-28-2 HCAPLUS
CN Technetium-99Tc, [2-(dimethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



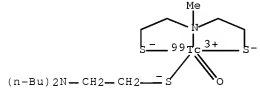
RN 178443-29-3 HCAPLUS
CN Technetium-99Tc, [2-(diethylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



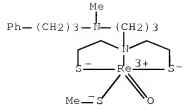
RN 178443-30-6 HCAPLUS
CN Technetium-99Tc, [8-(diethylamino)-1-octanethiolato-S][[2,2'-(methylimino)bis[ethanethiolato]](2-)-N,S,S']oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



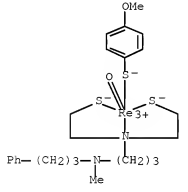
RN 178443-31-7 HCAPLUS
CN Technetium-99Tc, [2-(dibutylamino)ethanethiolato-κS][[2,2'-(methylimino-κN)bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 178443-47-5 HCAPLUS
CN Rhenium, (methanethiolato)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



RN 178443-48-6 HCAPLUS
CN Rhenium, (4-methoxybenzenethiolato-κS)[[2,2'-[[3-[methyl(3-phenylpropyl)amino]propyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (SP-5-34)- (9CI) (CA INDEX NAME)



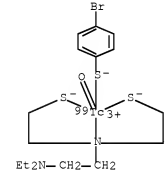
L13 ANSWER 49 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:121385 HCAPLUS Full-text
DOCUMENT NUMBER: 124:218510
ORIGINAL REFERENCE NO.: 124:40069a,40072a
TITLE: Synthesis and Characterization of Oxotechnetium(V) Mixed-Ligand Complexes Containing a Tridentate N-Substituted Bis(2-mercaptoethyl)amine and a Monodentate Thiol
AUTHOR(S): Pirmettis, I. C.; Papadopoulos, M. S.; Mastrostamatis, S. G.; Raptopoulou, C. P.; Terzis, A.; Chiotellis, E.
CORPORATE SOURCE: Institute of Radioisotopes-Radiodiagnostic Products, NCSR Demokritos, Aghia Paraskevi, 15310, Greece
SOURCE: Inorganic Chemistry (1996), 35(6), 1685-91
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 22 mixed-ligand complexes TcOL1L2, where L1H2 are N-substituted bis(2-mercaptoethyl)amine ligands, [SN(R)S], and L2H are monodentate thiols as coligand, is reported. The complexes were prepared by the ligand exchange method using Tc-gluconate as precursor and equimolar quantities of the two ligands. In all cases the syn stereoisomer was formed in high yield and isolated as a crystalline product. In four cases HPLC anal. demonstrated the presence of the anti stereoisomer in the reaction mixture Although the yield was <1%, one anti isomer was successfully isolated as brown crystals,

[TcO((SCH2CH2)2NCH2CH2NEt2)(S-p-C6H4OMe)]. The isolated complexes were characterized by spectroscopic methods and elemental anal. The formation of the two diastereomers, syn and anti, was expected due to the configuration of the nitrogen substituent (R) with respect to the central TcO core. The x-ray crystallog. showed that the coordination geometry of the syn isomers is trigonal bipyramidal while for the anti isomer is distorted square pyramidal. This is the 1st documentation of syn/anti isomerism in N-substituted TcO[SN(R)S][S] mixed-ligand complexes.

IT 174537-74-7P 174537-75-8P 174537-76-9P
174592-02-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure)

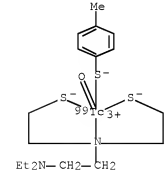
RN 174537-74-7 HCAPLUS

CN Technetium-99Tc, (4-bromobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)



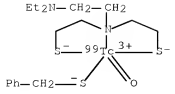
RN 174537-75-8 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

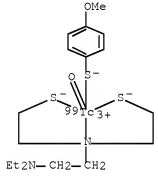


RN 174537-76-9 HCAPLUS

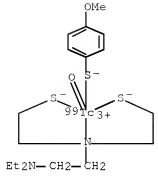
CN Technetium-99Tc, (benzenemethanethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



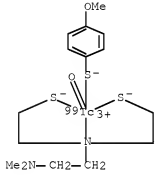
RN 174592-02-0 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, stereoisomer (9CI) (CA INDEX NAME)



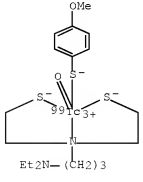
IT 158846-32-3P 174537-58-7P 174537-59-8P
174537-60-1P 174537-61-2P 174537-62-3P
174537-63-4P 174537-64-5P 174537-65-6P
174537-66-7P 174537-67-8P 174537-68-9P
174537-69-0P 174537-70-3P 174537-71-4P
174537-73-6P 174592-03-1P 174592-04-2P
174592-05-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 158846-32-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



RN 174537-58-7 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(dimethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

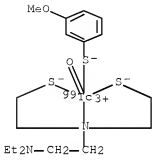


RN 174537-59-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[3-(diethylamino)propyl]imino]bis[ethanethiolato]](2-)](4-methoxybenzenethiolato-S)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)

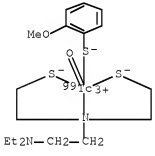


RN 174537-60-1 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-

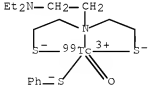
κN]bis[ethanethiolato-κS]](2-)](3-methoxybenzenethiolato-
κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



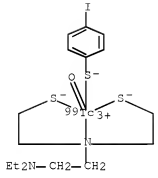
RN 174537-61-2 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)](2-methoxybenzenethiolato-
κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



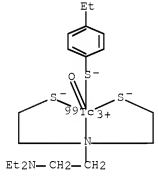
RN 174537-62-3 HCAPLUS
CN Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA
INDEX NAME)



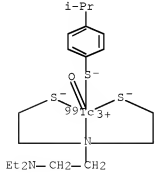
RN 174537-63-4 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-
κN]bis[ethanethiolato-κS]](2-)](4-iodobenzenethiolato-
κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



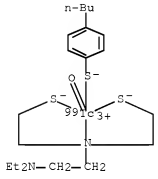
RN 174537-64-5 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-ethylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



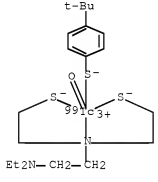
RN 174537-65-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1-methylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



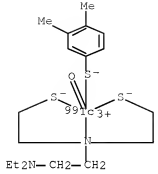
RN 174537-66-7 HCAPLUS
CN Technetium-99Tc, (4-butylbenzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



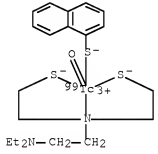
RN 174537-67-8 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenethiolato]oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



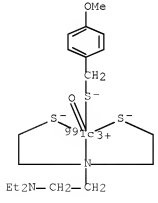
RN 174537-68-9 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](3,4-dimethylbenzenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



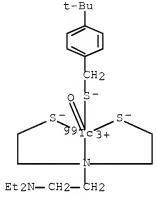
RN 174537-69-0 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](1-naphthalenethiolato)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



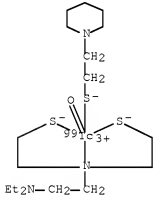
RN 174537-70-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenemethanethiolato-κS)oxo-, (TB-5-24)- (9CI) (CA INDEX NAME)



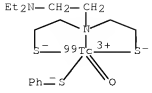
RN 174537-71-4 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenemethanethiolato]oxo-, stereoisomer (9CI) (CA INDEX NAME)



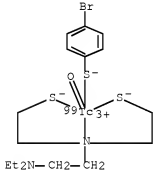
RN 174537-73-6 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino]bis[ethanethiolato]](2-)]oxo(1-piperidineethanethiolato-S)-, (TB-5-24)- (9CI) (CA INDEX NAME)



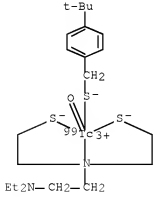
RN 174592-03-1 HCAPLUS
CN Technetium-99Tc, (benzenethiolato)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)



RN 174592-04-2 HCAPLUS
CN Technetium-99Tc, (4-bromobenzenethiolato-κS)[[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)]oxo-, stereoisomer (9CI) (CA INDEX NAME)



RN 174592-05-3 HCAPLUS
CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)][4-(1,1-dimethylethyl)benzenemethanethiolato]oxo-, stereoisomer (9CI) (CA INDEX NAME)



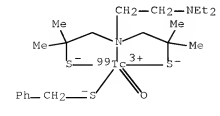
OS.CITING REF COUNT: 49 THERE ARE 49 CAPLUS RECORDS THAT CITE THIS RECORD (49 CITINGS)

L13 ANSWER 50 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:380681 HCAPLUS Full-text
DOCUMENT NUMBER: 122:150064
ORIGINAL REFERENCE NO.: 122:27514h,27515a
TITLE: Synthesis and Characterization of Oxotechnetium(V) Complexes with Aza-Substituted 2,6-Dimethyl-4-azaheptane-2,6-dithiol Ligands and Benzyl Mercaptan as Coligand
AUTHOR(S): Spyriounis, D. M.; Pelecanou, M.; Stassinopoulou, C. I.; Raptopoulou, C. P.; Terzis, A.; Chiotellis, E.
CORPORATE SOURCE: Institutes of Radioisotopes-Radiodiagnostic Products Biology, Athens, Greece
SOURCE: Inorganic Chemistry (1995), 34(5), 1077-82
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The design and synthesis of mixed oxotechnetium(V)-99 complexes with aza-substituted 2,6-dimethyl-4-azaheptane-2,6-dithiol ligands NS2 and benzyl mercaptan as coligand are reported. Ligands (general formula R-CH2CH2N[CH2CMe2SH]2 with R = NEt2, piperidin-1-yl, pyrrolidin-1-yl, and morpholin-4-yl) were synthesized through the reduction of aza-substituted heterocyclic aza disulfides which result from the reductive cyclization of 2,2'-dithiobis(2-methylpropanal) with the appropriate primary amine. The 99Tc complexes, TcO{[SCMe2CH2]2NCH2CH2R}X (5; X = benzyl mercaptan), were prepared in high yield by the reaction of 99Tc(V) gluconate with a 1:1 mixture of the appropriate tris-chelating ligand and the monodentate benzyl mercaptan. The resulting complexes were purified through flash column chromatog. Crystals were formed by dissolving complexes in a mixture of MeOH/water and slowly evaporating the solvents. Complexes were characterized by elemental analyses and spectroscopic methods. Complete assignments of 1H and 13C NMR resonances were made for all complexes. X-ray crystallog. anal. of 5d (C21H35N2S3O2Tc, R = morpholin-4-yl) showed that the complex crystallizes in the monoclinic space group P21/c with a 17.166(2), b 8.9282(7), c 17.738(2) Å, β 116.031(3)°, and Z = 4. Complex 5d has trigonally distorted square pyramidal coordination geometry around technetium with the side chain on nitrogen directed toward the oxygen of the Tc:O core (syn configuration). The nOe data confirm that in all cases the major isolated product of the synthesis has the syn configuration of the side chain.

IT 160297-81-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR spectra)
RN 160297-81-4 HCAPLUS
CN Technetium-99Tc, (benzenemethanethiolato)[[1,1'-[[2-(diethylamino)ethyl]imino]bis[2-methyl-2-propanethiolato]](2-)]oxo-, (SP-5-31)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 40 THERE ARE 40 CAPLUS RECORDS THAT CITE THIS

RECORD (40 CITINGS)

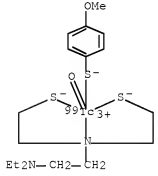
L13 ANSWER 51 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:140207 HCAPLUS Full-text
DOCUMENT NUMBER: 122:70327
ORIGINAL REFERENCE NO.: 122:13147a,13150a
TITLE: 1H and 13C NMR structural studies in solution of oxotechnetium(V) complexes with N,N-bis(2-mercaptoethyl)-N',N'-diethylethylenediamine and N,N-bis(2-mercaptoethyl)-2-ethylthioethylamine
AUTHOR(S): Stassinopoulou, C. I.; Pelecanou, M.; Mastrostamatis, S.; Chiotellis, E.
CORPORATE SOURCE: Inst. Biol., NCSR 'Demokritos", Paraskevi, Greece
SOURCE: Magnetic Resonance in Chemistry (1994), 32(9), 532-6
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The complete assignments of the 1H and 13C resonances of 3 TcOLX complexes of oxotechnetium(V)-99 with H2L = N,N-bis(2-mercaptoethyl)-N',N'-diethylethylenediamine or N,N-bis(2-mercaptoethyl)-2-ethylthioethylamine and X = p-methoxythiophenolate or chloride ions are reported. Chemical shifts are influenced by the proximity of protons and carbons to the coordinated heteroatoms and by their orientation with respect to the Tc:O core. The NMR spectra at room temperature are the result of motionally averaged conformations.

IT 158846-32-3
RL: PRP (Properties)
(1H and 13C NMR structural studies of)

RN 158846-32-3 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L13 ANSWER 52 OF 52 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:691268 HCAPLUS Full-text
DOCUMENT NUMBER: 121:291268
ORIGINAL REFERENCE NO.: 121:52983a,52986a
TITLE: Tridentate ligands containing the SNS donor atom set

as a novel backbone for the development of technetium brain-imaging agents

AUTHOR(S): Mastrostamatis, Spiros G.; Papadopoulos, Minas S.; Pirmettis, Ioannis C.; Paschali, Evagelia; Varvarigou, Alexandra D.; Stassinopoulou, Chariklia I.; Raptopoulou, Cathrine P.; Terzis, Aris; Chiotellis, Efstratios

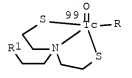
CORPORATE SOURCE: Institute of Radioisotopes-Radiodiagnostic Products Biology, NCSR Demokritos, Aghia Paraskevi, 153 10, Greece

SOURCE: Journal of Medicinal Chemistry (1994), 37(20), 3212-18
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



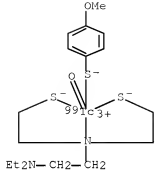
I

AB In developing 99mTc complexes as potential brain-imaging agents, we investigated the coordination chemical of ligands containing sulfur and nitrogen donor atoms with the general formula R-CH2CH2N(CH2CH2SH)2 (R = EtS, Et2N). These ligands act as tridentate SNS chelates to the TcO3+ core, leaving open one coordination site cis to the oxo group. In reactions with the highly reactive [99TcOCl4]- precursor, this vacancy was occupied by a chlorine atom. When the ligands reacted in the presence of 4-methoxythiophenol, using 99Tc(V)-gluconate as precursor, the vacancy was filled with 4-methoxythiophenol, which acted as co-ligand. Thus neutral mixed ligand complexes of the general formula I (R = Cl, R1 = SEt (II), R = SC6H4)Me-4, R1 = SEt (III), NEt2 (IV), were synthesized. The complexes were characterized by UV, IR, 1H NMR, crystallog., and elemental analyses. The crystal structures of II and IV demonstrated that the coordination geometry is trigonal bipyramidal with the N1 and Cl or S3 occupying the apical positions and the basal plane defined by the S1 and S2 of the tridentate ligand and the oxo group. The complexes III(99mTc) and IV(99mTc) were prepared using 99mTc-glucoheptonate as precursor and were purified by HPLC. Biodistribution in mice showed high initial brain uptake (3.68% and 3.56% dose/organ for III(99mTc) and IV(99mTc), resp.). Complex IV(99mTc) displayed significantly higher brain/blood values and prolonged retention in brain as well. The results suggest that structural modifications based on configurations III-IV may provide novel 99mTc brain-imaging agents with improved biol. characteristics.

IT 158846-32-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of, as a novel backbone for technetium brain-imaging agents)

RN 158846-32-3 HCAPLUS

CN Technetium-99Tc, [[2,2'-[[2-(diethylamino)ethyl]imino-κN]bis[ethanethiolato-κS]](2-)](4-methoxybenzenethiolato-κS)oxo-, (TB-5-14)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 44 THERE ARE 44 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)

=>
=>